

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
 Data File : BP007040.D
 Acq On : 17 Sep 2021 23:02
 Operator : CG/JU
 Sample : M3791-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-RR-02-(1.0)

Integration Parameters: rteint.p

Integrator: RTE

Smothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007040.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.316	204	209	217	rBV	193622	287570	1.63%	0.255%
2	4.669	240	269	270	rBV6	95181	634164	3.58%	0.562%
3	4.728	275	279	282	rVV	201203	357578	2.02%	0.317%
4	4.799	283	291	305	rVB	286447	779921	4.41%	0.691%
5	5.022	324	329	340	rVB	209438	326588	1.85%	0.289%
6	5.481	400	407	416	rBV	1715869	2536613	14.34%	2.248%
7	7.069	670	677	689	rBV	991815	1641161	9.28%	1.454%
8	7.905	809	819	828	rBV	1228953	1977755	11.18%	1.752%
9	8.669	941	949	956	rBV	394937	658423	3.72%	0.583%
10	9.069	1003	1017	1026	rBV	3241883	5377575	30.40%	4.765%
11	9.393	1052	1072	1079	rBV	740069	2607057	14.74%	2.310%
12	9.628	1106	1112	1119	rVB3	100671	183669	1.04%	0.163%
13	9.946	1156	1166	1175	rBV	100288	221861	1.25%	0.197%
14	10.151	1191	1201	1210	rBV	1960168	3423297	19.35%	3.033%
15	10.487	1251	1258	1269	rBV	1803666	2849654	16.11%	2.525%
16	10.704	1287	1295	1300	rBV	1618662	2722109	15.39%	2.412%
17	10.757	1300	1304	1310	rVB	417008	692002	3.91%	0.613%
18	11.246	1379	1387	1402	rBV	325825	692606	3.92%	0.614%
19	11.975	1506	1511	1522	rVB	107109	214060	1.21%	0.190%
20	12.398	1569	1583	1595	rBV	2695581	5595535	31.63%	4.958%
21	12.557	1595	1610	1633	rVB	2417566	7427219	41.98%	6.581%
22	13.163	1706	1713	1724	rBV	8617662	12738732	72.01%	11.287%
23	13.328	1735	1741	1754	rBV	221936	385566	2.18%	0.342%
24	13.440	1754	1760	1765	rVV	383632	593589	3.36%	0.526%
25	13.492	1765	1769	1780	rVB	261695	410107	2.32%	0.363%
26	14.534	1934	1946	1955	rBV	2384981	3670499	20.75%	3.252%
27	14.922	2007	2012	2022	rBV4	125280	255038	1.44%	0.226%
28	15.410	2089	2095	2100	rBV2	181599	267887	1.51%	0.237%
29	15.739	2142	2151	2157	rBV	119872	219343	1.24%	0.194%
30	15.910	2176	2180	2184	rBV	273488	351377	1.99%	0.311%
31	16.016	2192	2198	2206	rVB	4354495	6314825	35.70%	5.595%
32	16.198	2219	2229	2234	rBV	204235	431324	2.44%	0.382%
33	16.286	2239	2244	2253	rVB	768755	1087492	6.15%	0.964%
34	16.363	2253	2257	2263	rBV	847164	1080740	6.11%	0.958%
35	16.786	2321	2329	2344	rBV	3250772	5692790	32.18%	5.044%
36	17.280	2407	2413	2417	rBV	2858627	4104880	23.20%	3.637%

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Instrument :
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SW-RR-02-(1.0)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
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37	17.328	2417	2421	2426	rVB2	411964	602368	3.41%	0.534%
38	17.498	2446	2450	2461	rVB3	174560	339818	1.92%	0.301%
39	17.657	2472	2477	2486	rVB3	139974	229504	1.30%	0.203%
40	17.951	2523	2527	2532	rBV	249080	298141	1.69%	0.264%
41	18.169	2559	2564	2573	rBV	563460	898442	5.08%	0.796%
42	19.080	2716	2719	2727	rVB	804535	918505	5.19%	0.814%
43	19.210	2738	2741	2746	rVB	251763	286862	1.62%	0.254%
44	19.398	2769	2773	2780	rBV	328826	420648	2.38%	0.373%
45	19.833	2842	2847	2858	rBV	14264754	17690610	100.00%	15.675%
46	21.045	3049	3053	3055	rBV2	269413	355966	2.01%	0.315%
47	21.069	3055	3057	3065	rVB2	413075	472090	2.67%	0.418%
48	21.357	3101	3106	3116	rBV	3614063	4672284	26.41%	4.140%
49	23.468	3461	3465	3477	rVB3	412949	778736	4.40%	0.690%
50	23.768	3510	3516	3533	rVB2	2299088	4875198	27.56%	4.320%
51	24.986	3718	3723	3736	rVB3	529280	1209111	6.83%	1.071%

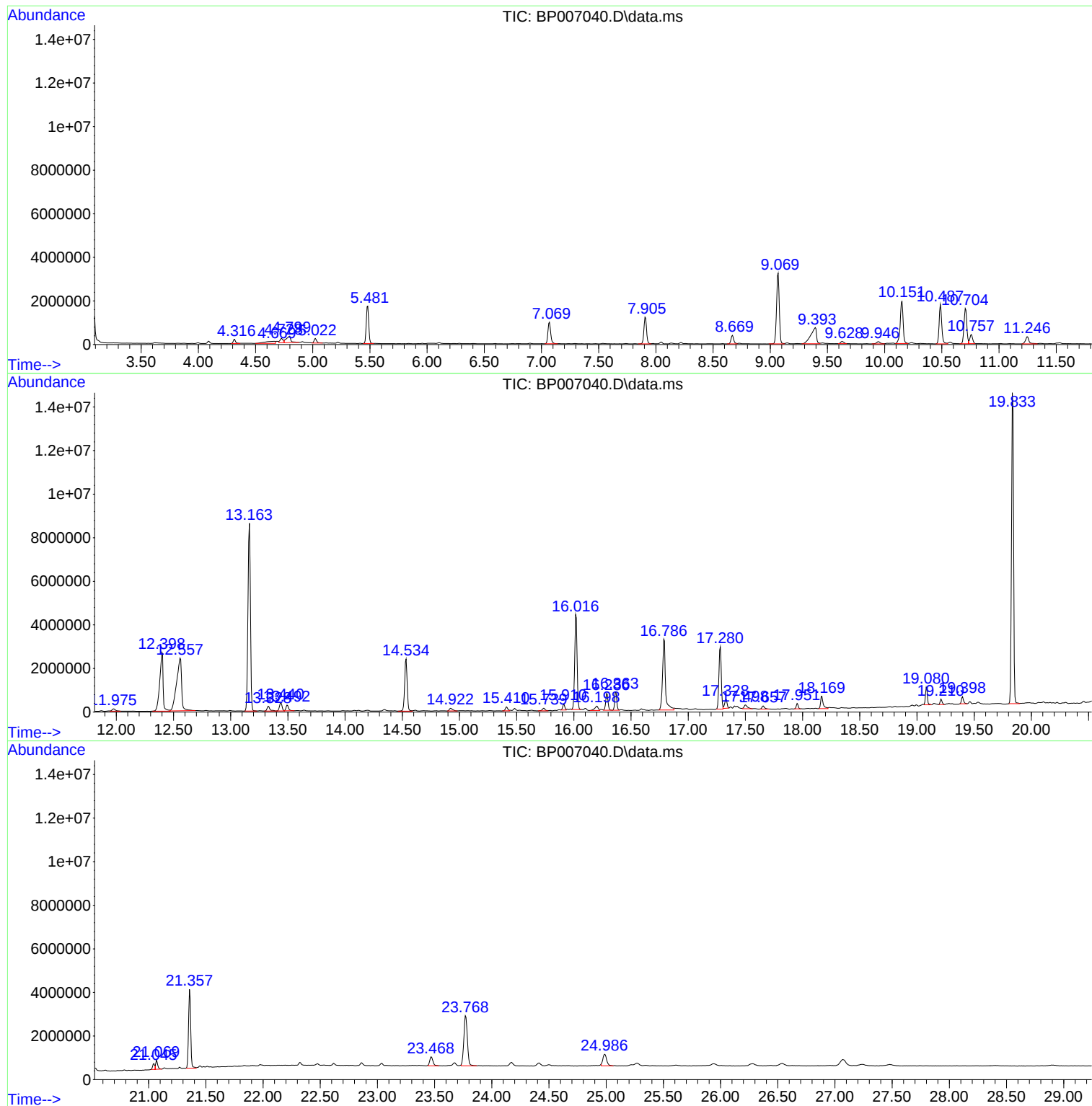
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

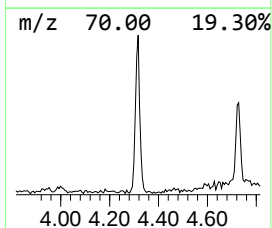
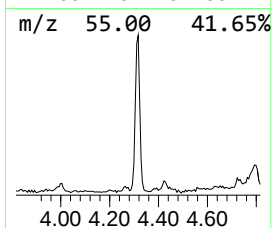
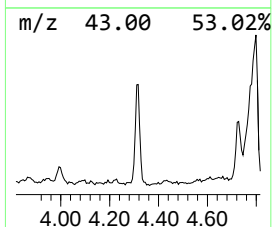
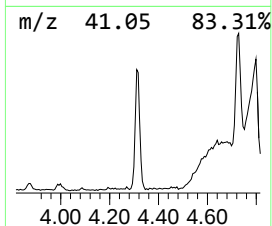
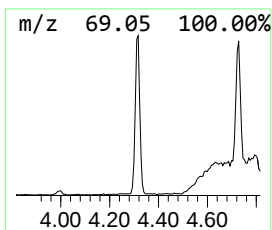
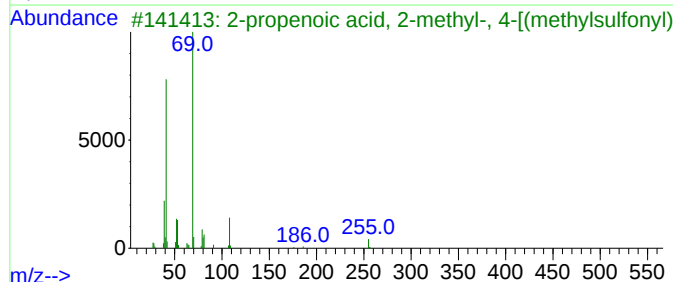
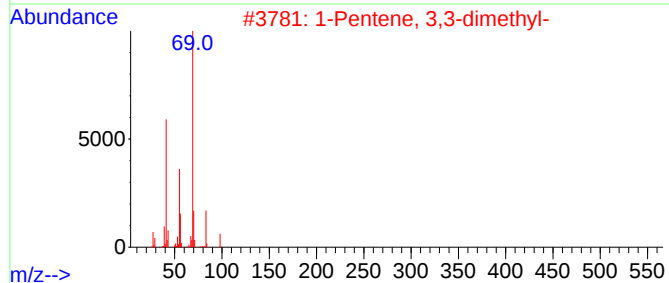
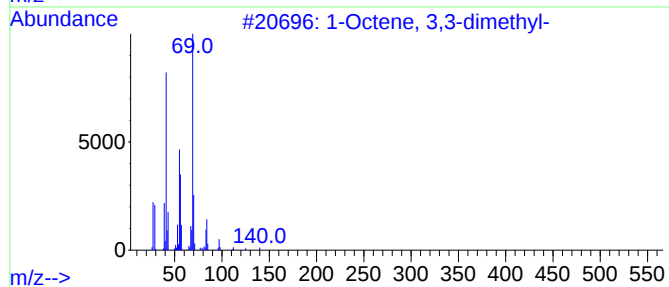
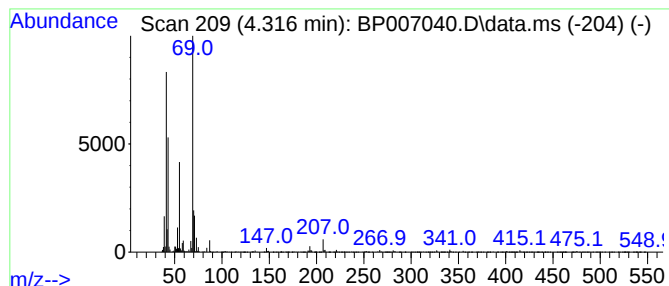
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.316 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.316	2.91 ng	287570	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 3,3-dimethyl-			140	C10H20	074511-51-6	45
2	1-Pentene, 3,3-dimethyl-			98	C7H14	003404-73-7	45
3	2-propenoic acid, 2-methyl-, 4-[...]			255	C11H13NO4S	1000401-46-9	38
4	2-Butenoic acid, 4-nitrophenyl e...			207	C10H9NO4	014617-88-0	36
5	1-Pentyn-1-ol, 4-methyl-			98	C6H10O	053778-57-7	28



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Instrument :
BNA_P
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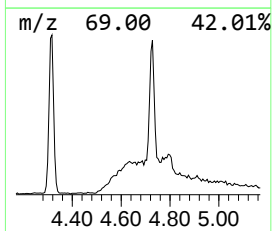
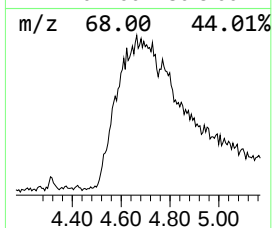
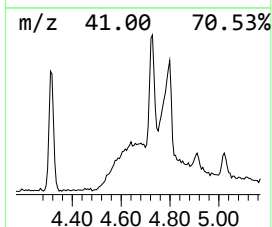
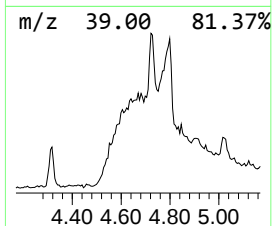
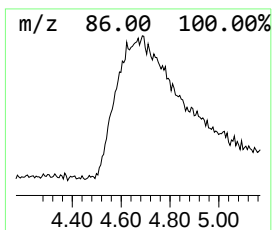
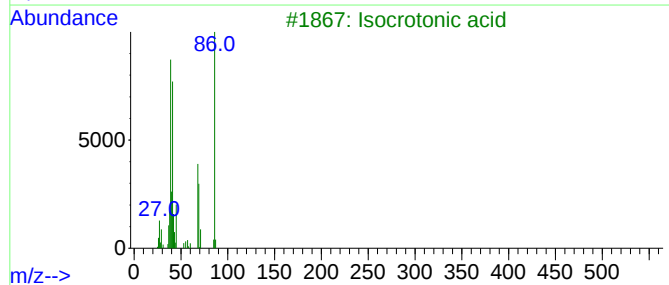
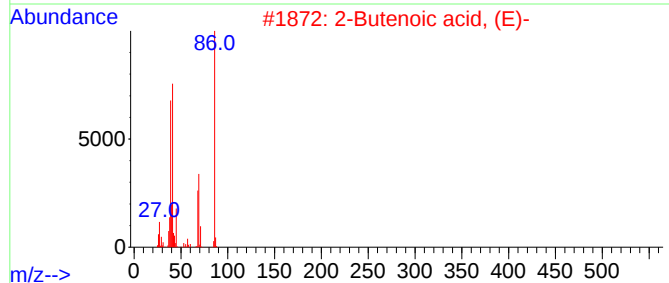
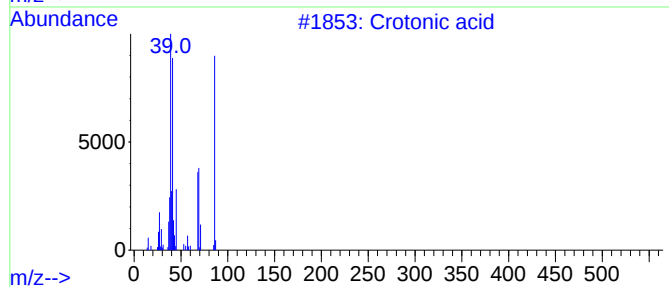
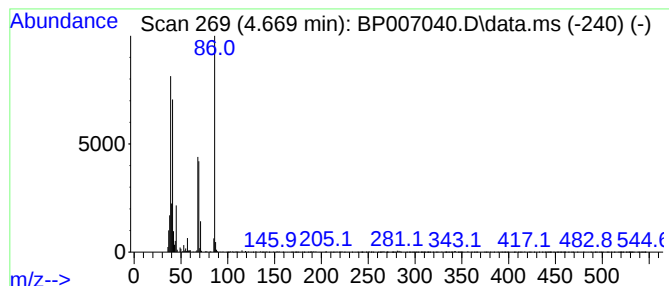
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Crotonic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.669	6.41 ng	634164	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Crotonic acid	86	C4H6O2	003724-65-0	95
2			2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	91
3			Isocrotonic acid	86	C4H6O2	000503-64-0	91
4			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	90
5			2-Butenedioic acid, 2-methyl-, (Z)-	130	C5H6O4	000498-23-7	78



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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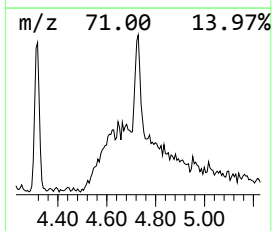
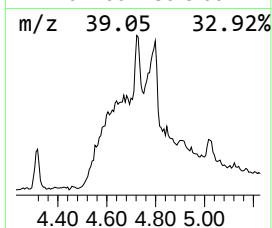
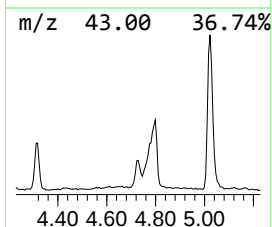
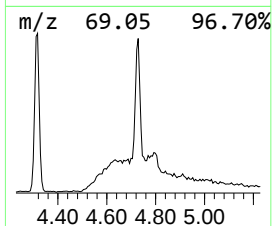
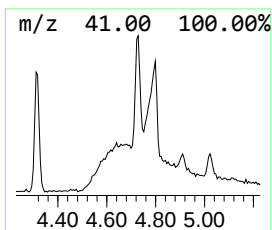
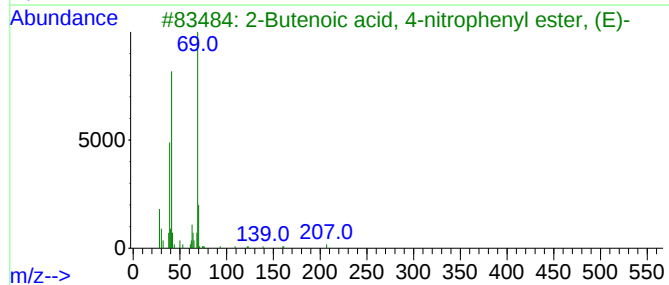
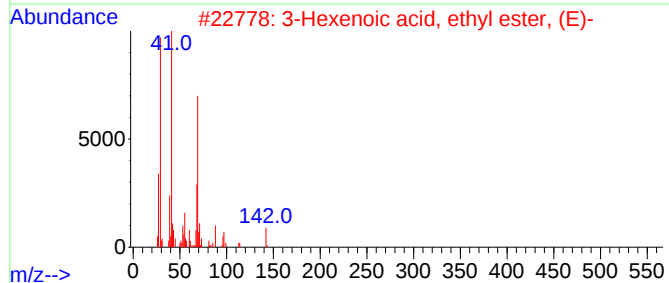
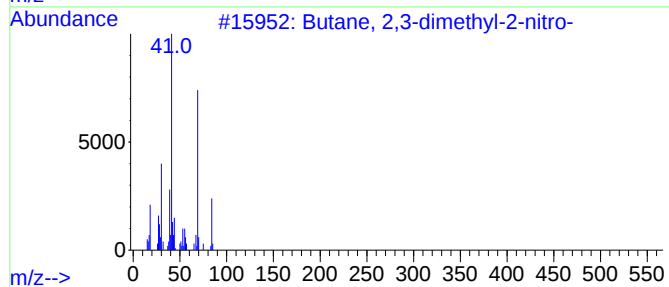
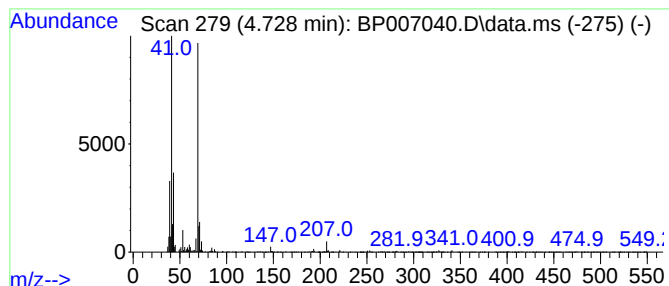
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2,3-dimethyl-2-nitro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.728	3.62 ng	357578	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	53
2			3-Hexenoic acid, ethyl ester, (E)-	142	C8H14O2	026553-46-8	45
3			2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	42
4			3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	42
5			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	42



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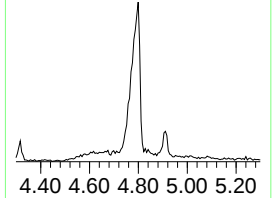
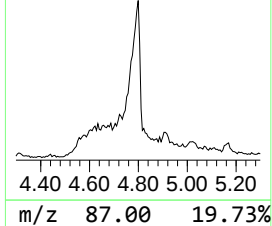
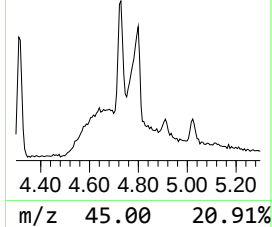
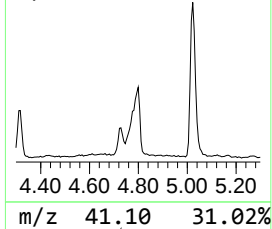
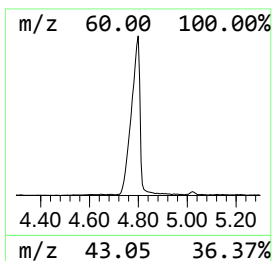
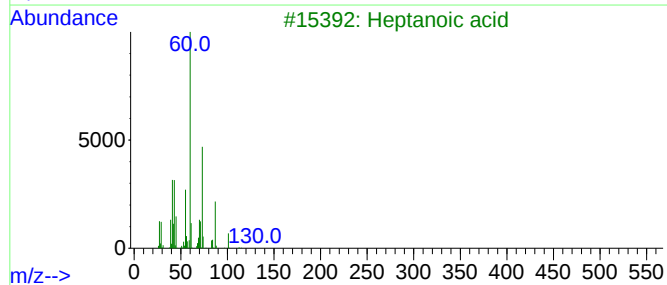
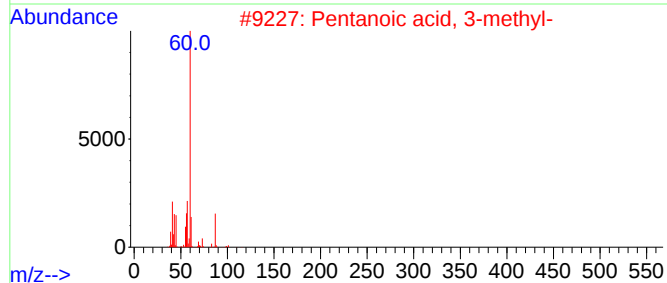
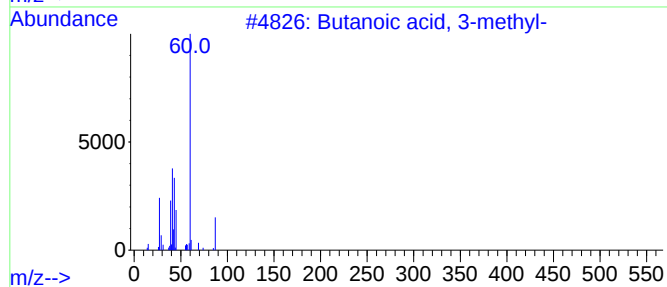
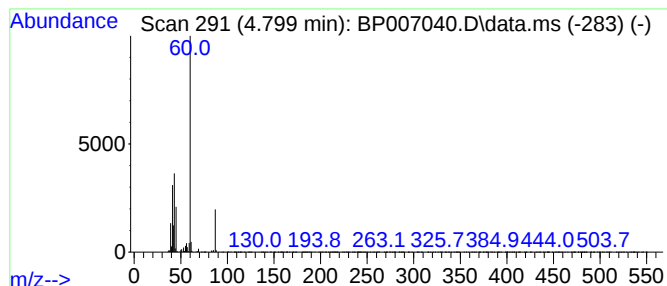
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.799	7.89 ng	779921	1,4-Dichlorobenzene-d4	7.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	72
3	Heptanoic acid	130	C7H14O2	000111-14-8	39
4	Pentanoic acid	102	C5H10O2	000109-52-4	36
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	28



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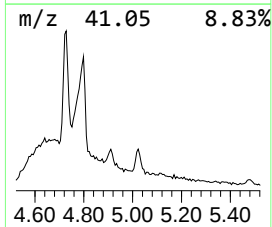
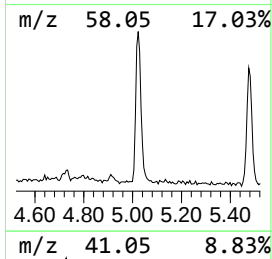
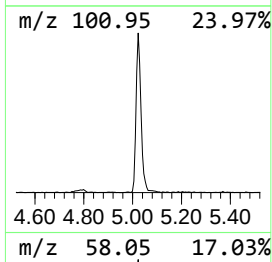
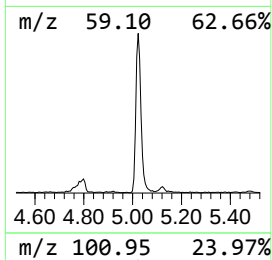
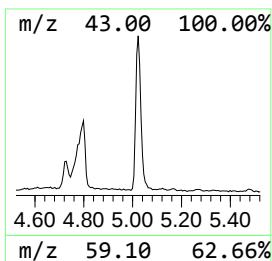
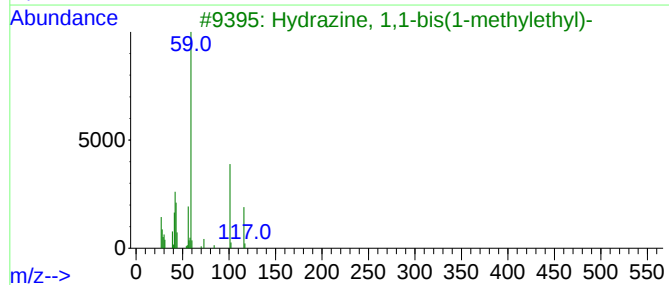
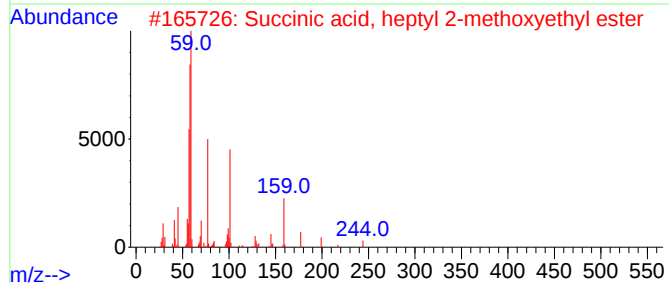
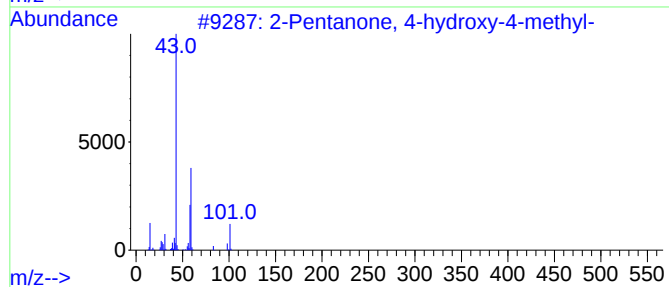
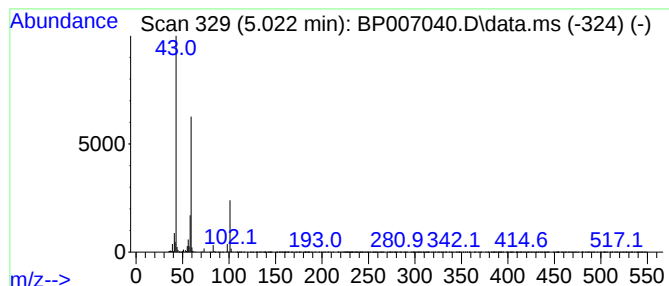
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.30 ng	326588	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

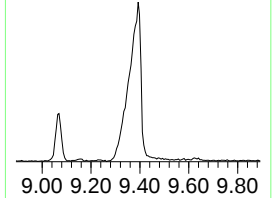
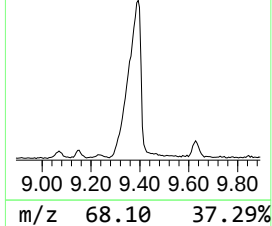
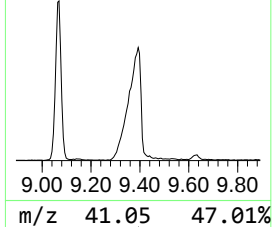
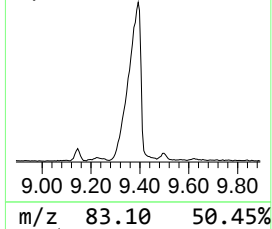
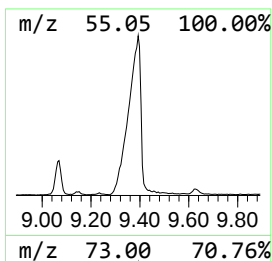
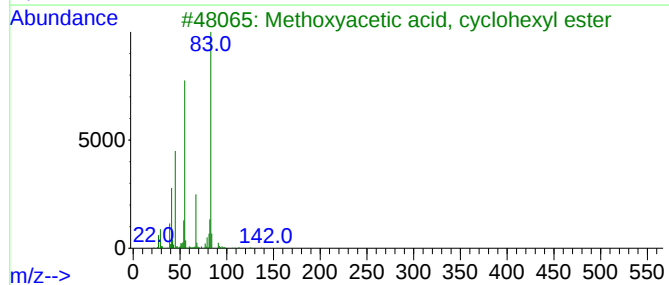
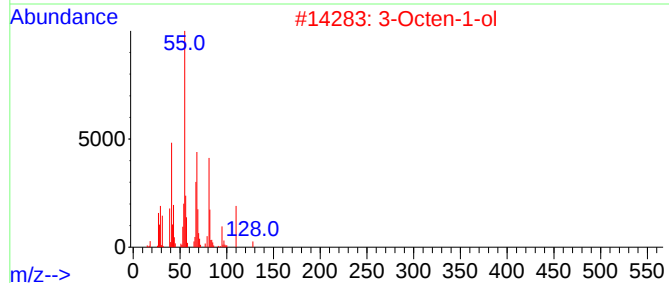
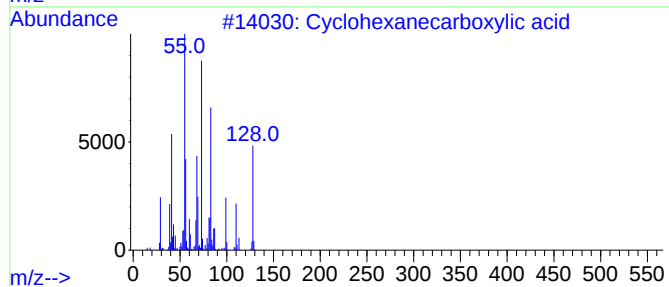
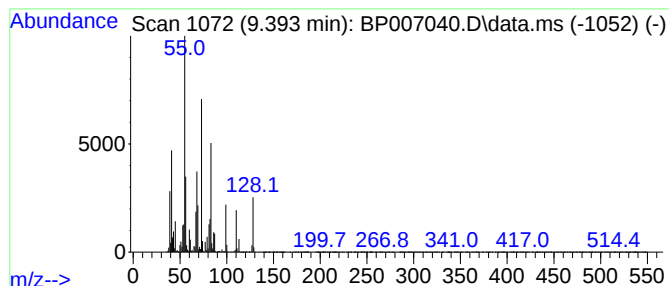
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexanecarboxylic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.393	19.15 ng	2607060	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	97
2			3-Octen-1-ol	128	C8H16O	018185-81-4	35
3			Methoxyacetic acid, cyclohexyl e...	172	C9H16O3	1000282-69-4	22
4			Ethyl 1-methylcyclopropanecarbox...	128	C7H12O2	071441-76-4	22
5			1-Cyclohexylethanol, trifluoroac...	224	C10H15F3O2	1000365-19-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

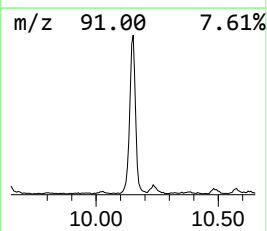
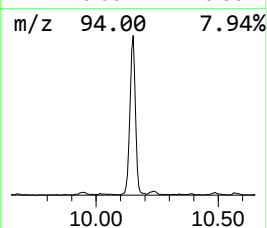
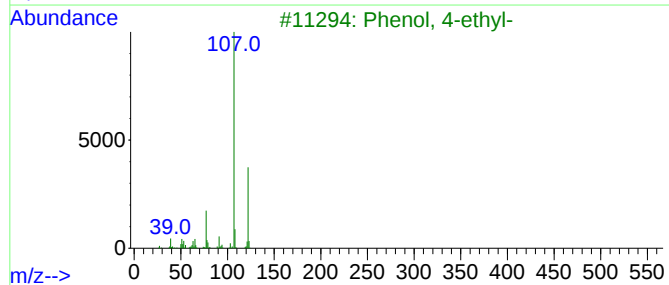
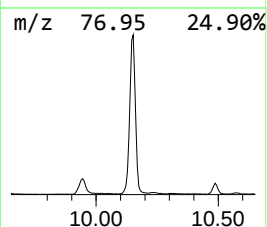
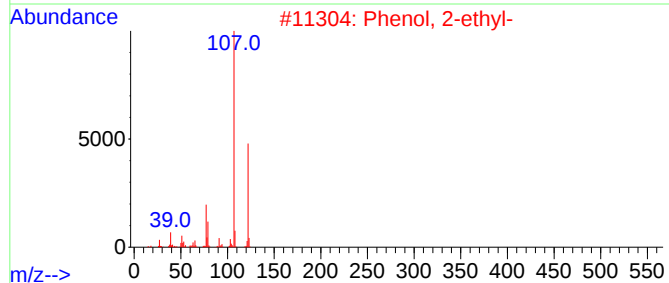
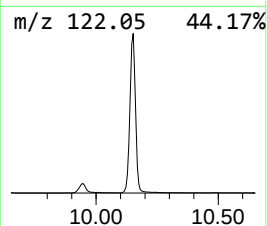
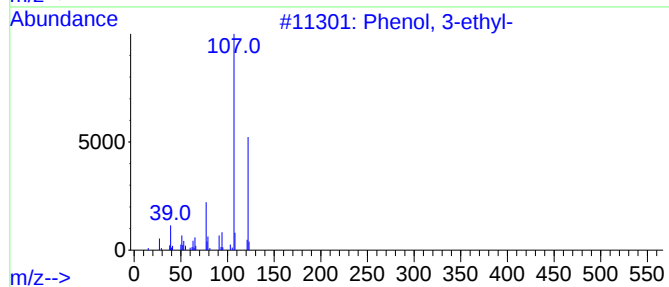
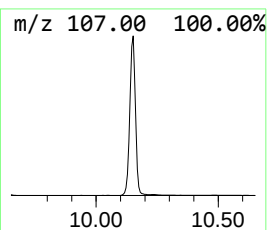
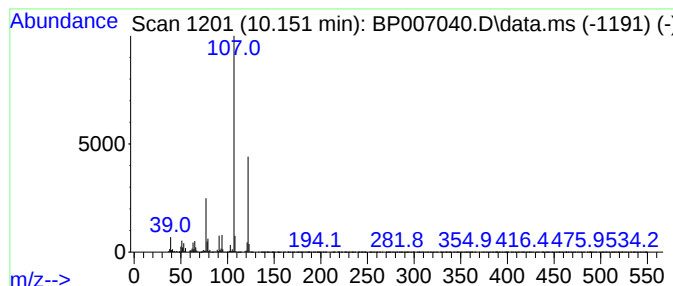
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Phenol, 3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.152	25.15 ng	3423300	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 3-ethyl-	122	C8H10O	000620-17-7	97
2			Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3			Phenol, 4-ethyl-	122	C8H10O	000123-07-9	90
4			Silane, 1,3-butadiynyltrimethyl-	122	C7H10Si	004526-06-1	59
5			2-Isopropylpyrazine	122	C7H10N2	029460-90-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

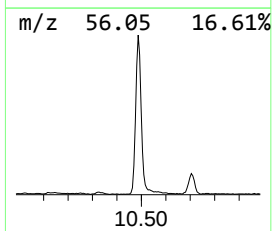
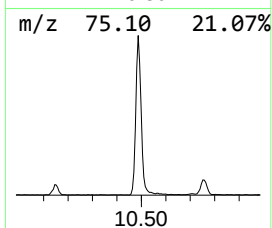
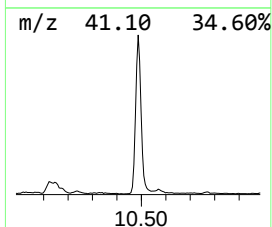
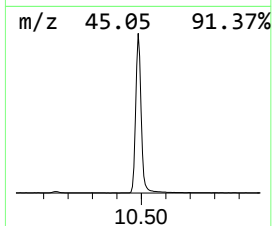
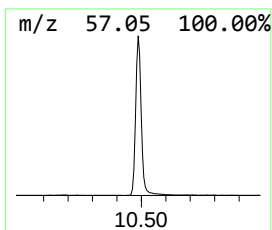
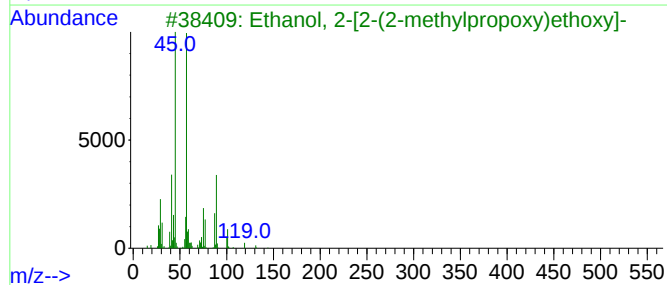
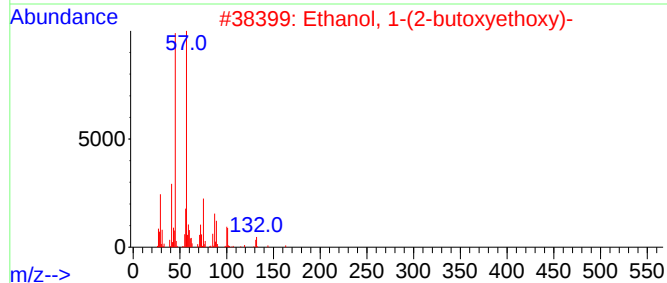
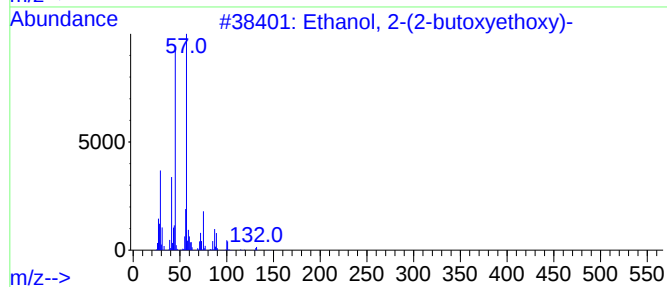
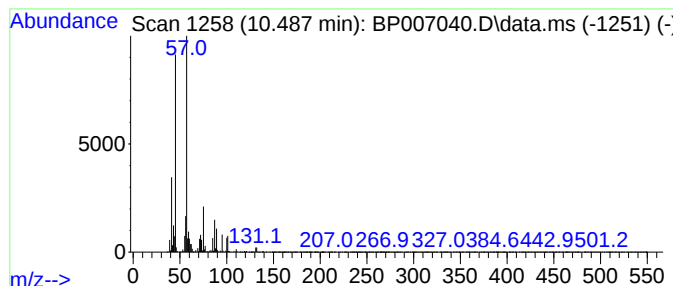
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	20.94 ng	2849650	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

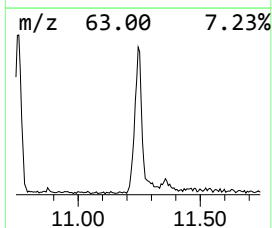
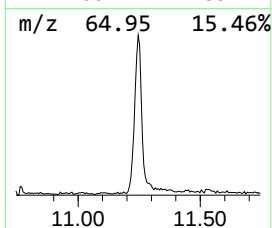
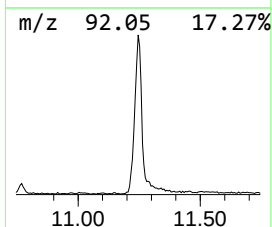
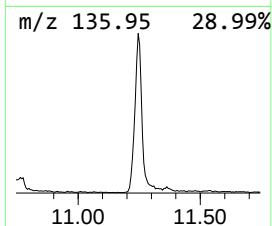
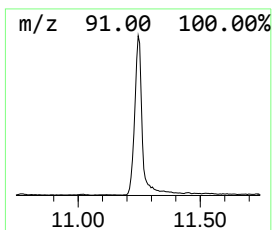
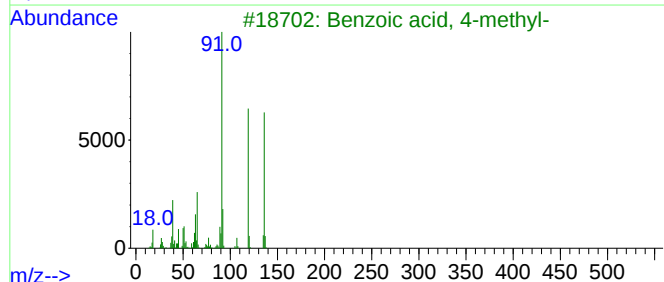
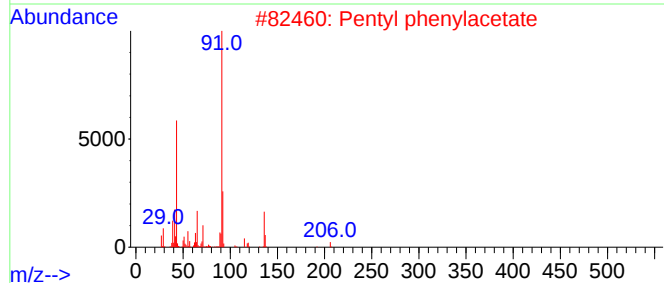
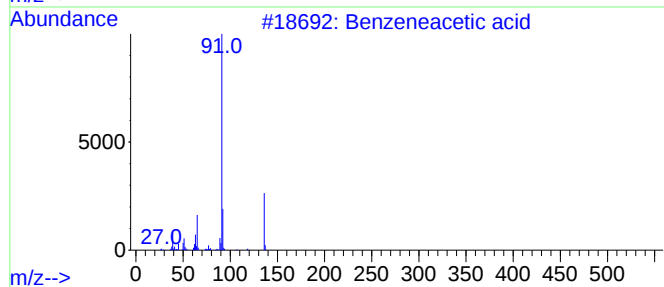
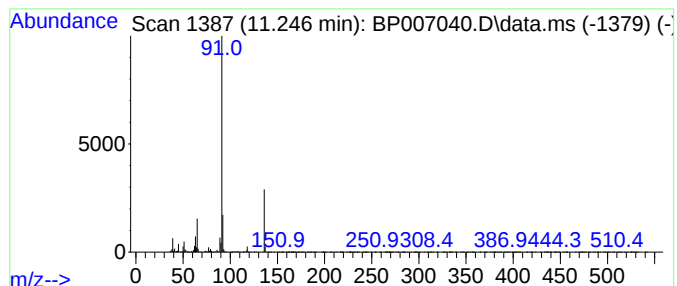
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzeneacetic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.246	5.09 ng	692606	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	94
2			Pentyl phenylacetate	206	C13H18O2	005137-52-0	59
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	58
4			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	50
5			3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

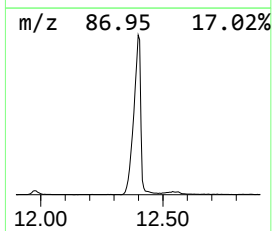
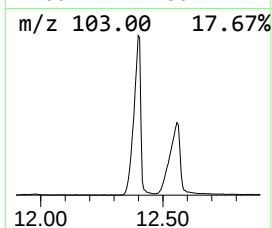
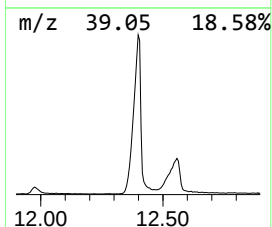
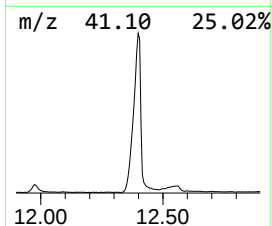
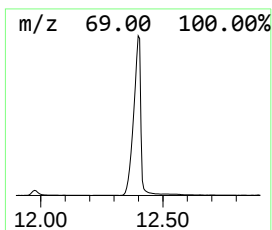
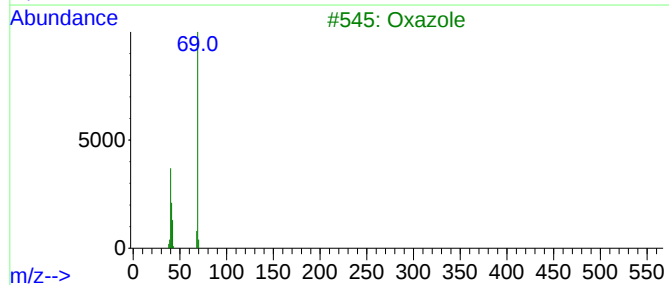
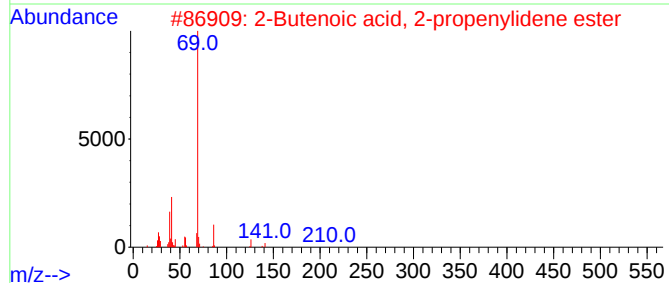
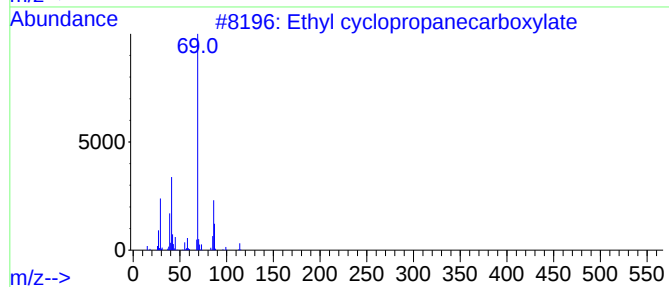
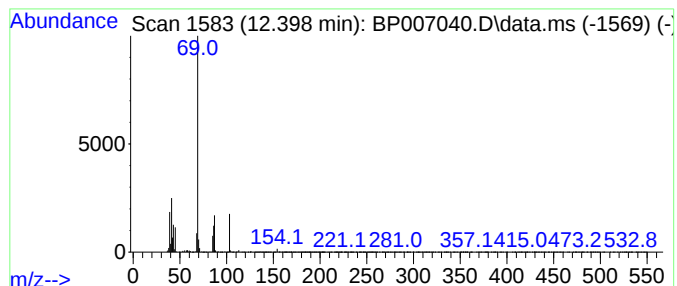
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown12.398 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	41.11 ng	5595540	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
3			Oxazole	69	C3H3NO	000288-42-6	9
4			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
5			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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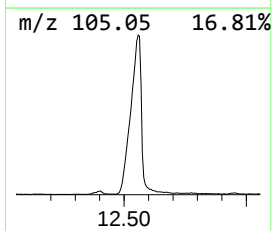
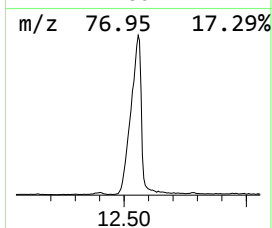
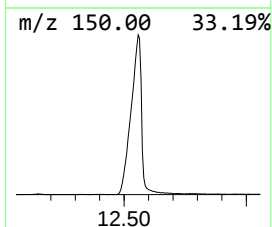
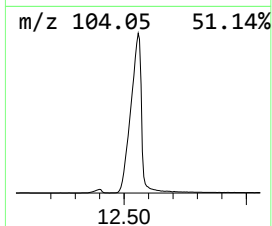
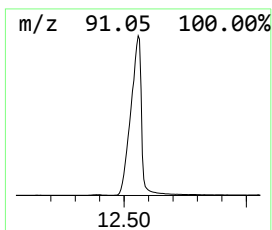
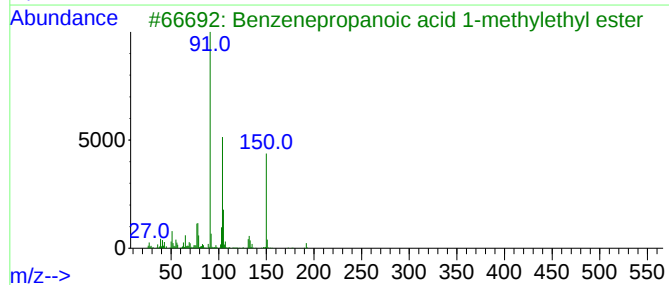
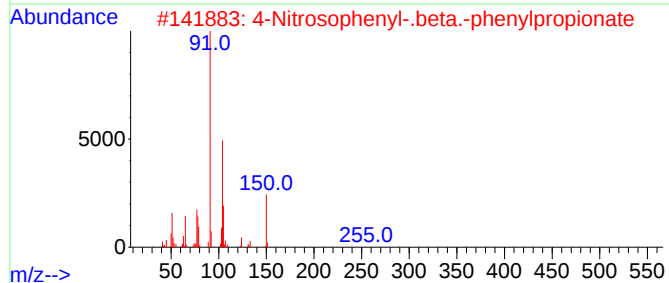
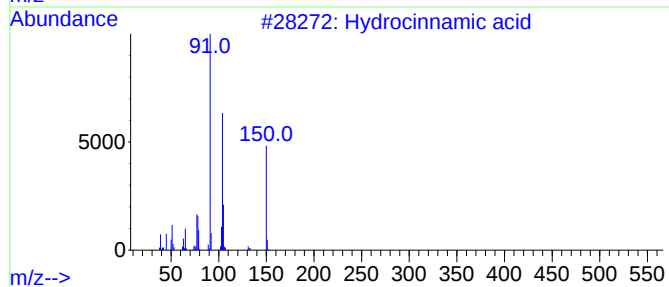
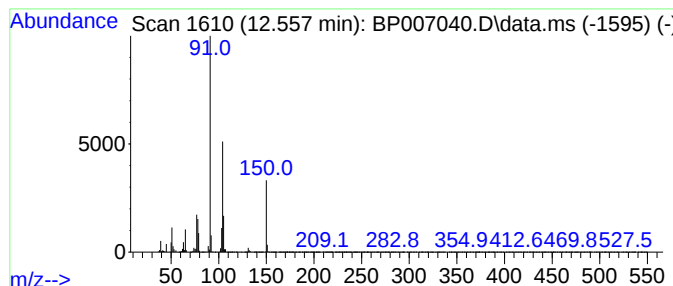
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hydrocinnamic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	54.57 ng	7427220	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	97
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3			Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	78
4			Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	50
5			Propanoic acid, 2,2-dimethyl-, 2...	206	C13H18O2	067662-96-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

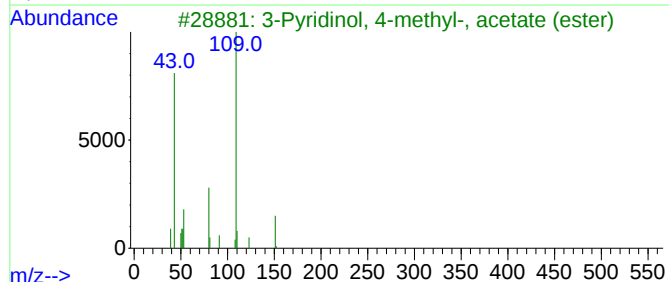
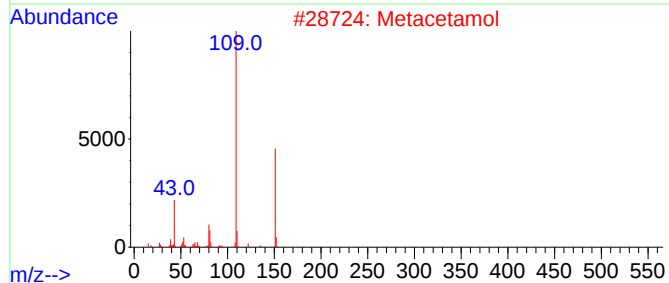
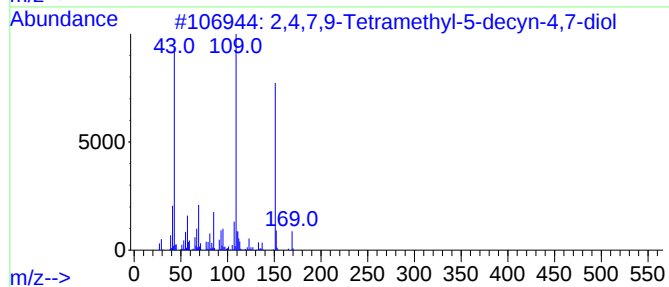
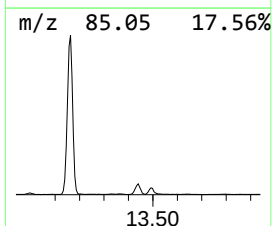
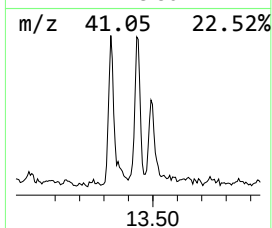
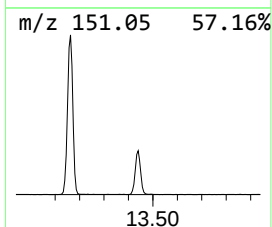
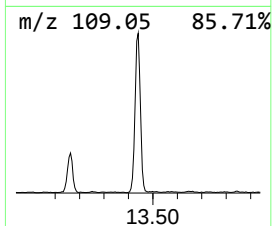
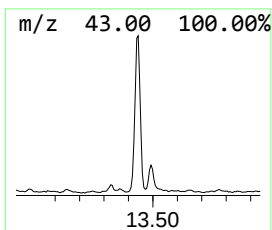
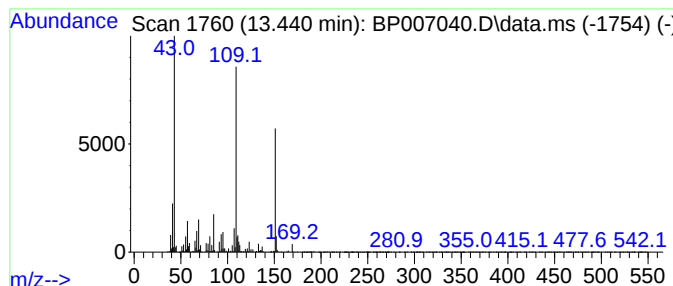
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ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.440	3.23 ng	593589	Acenaphthene-d10	14.534	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	53
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
4	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	43
5	4-(1,5-Dihydroxy-2,6,6-trimethyl...	224	C13H20O3	1000191-85-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

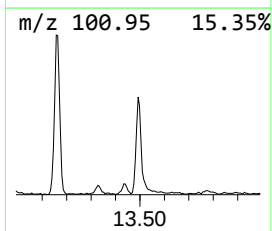
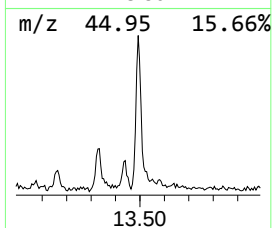
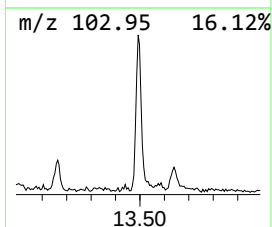
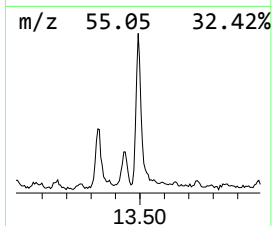
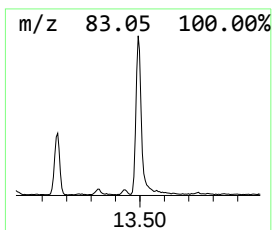
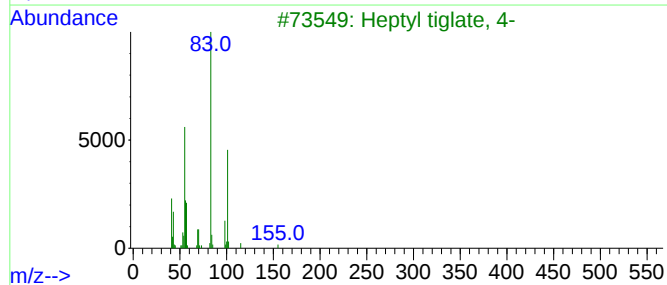
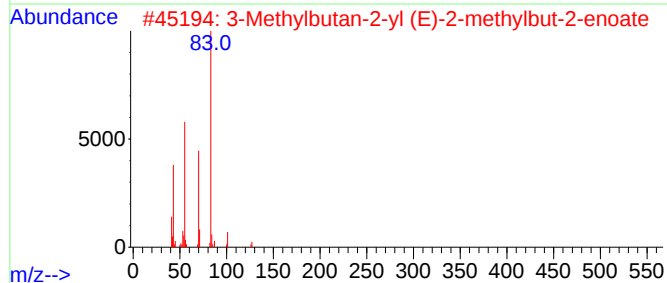
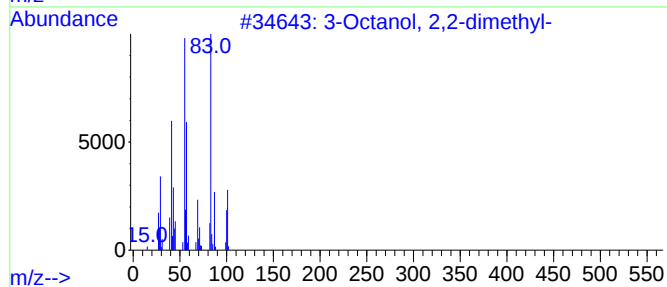
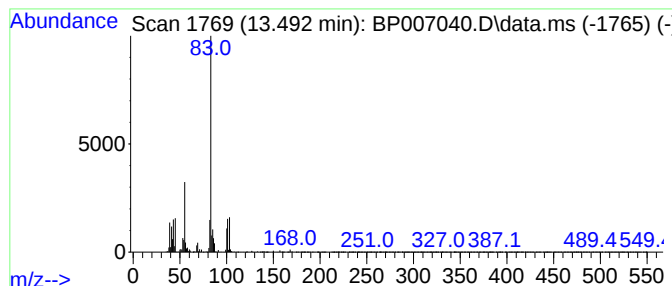
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 3-Octanol, 2,2-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.493	2.23 ng	410107	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanol, 2,2-dimethyl-	158	C10H22O	019841-72-6	59
2			3-Methylbutan-2-yl (E)-2-methylb...	170	C10H18O2	1000373-73-4	53
3			Heptyl tiglate, 4-	198	C12H22O2	1000383-64-0	50
4			Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	50
5			2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

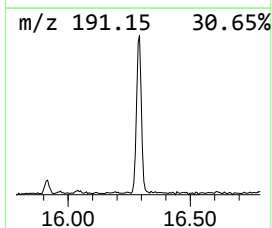
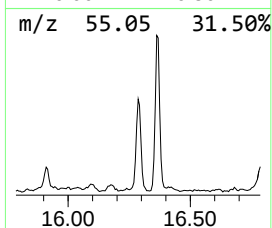
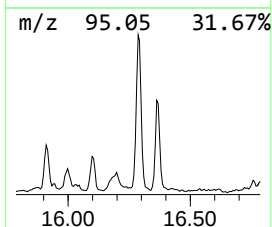
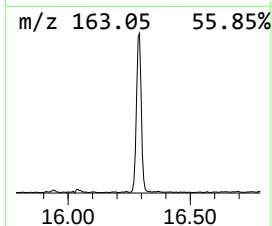
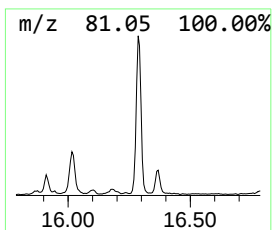
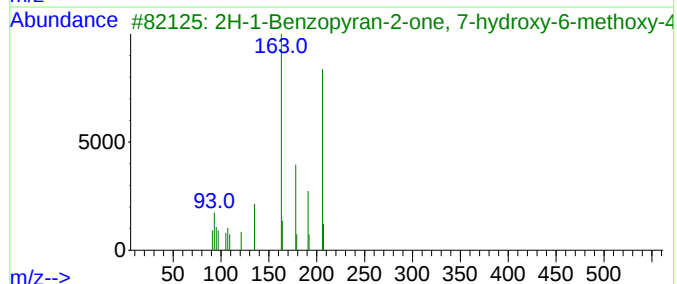
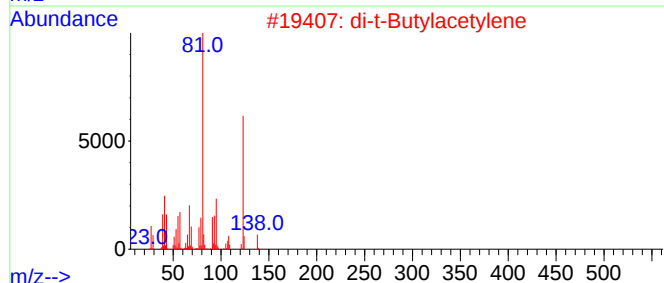
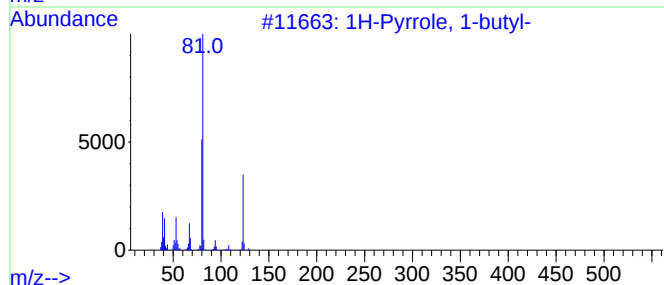
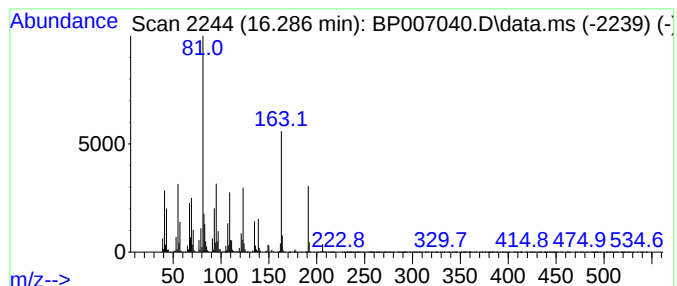
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown16.286 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.286	5.30 ng	1087490	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	35
2			di-t-Butylacetylene	138	C10H18	017530-24-4	32
3			2H-1-Benzopyran-2-one, 7-hydroxy...	206	C11H10O4	003374-03-6	32
4			2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	27
5			16-Heptadecyn-4-one, 1,2-dihydroxy-	282	C17H30O3	1379770-10-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

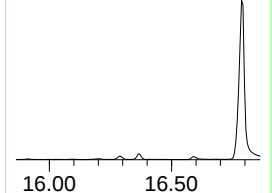
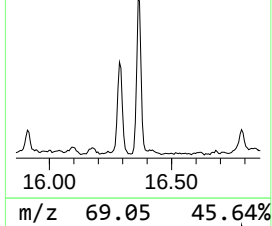
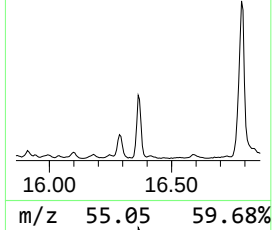
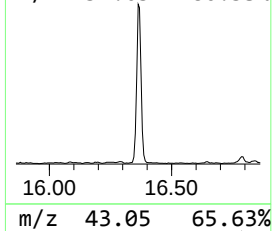
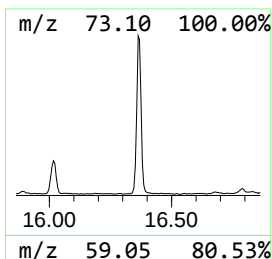
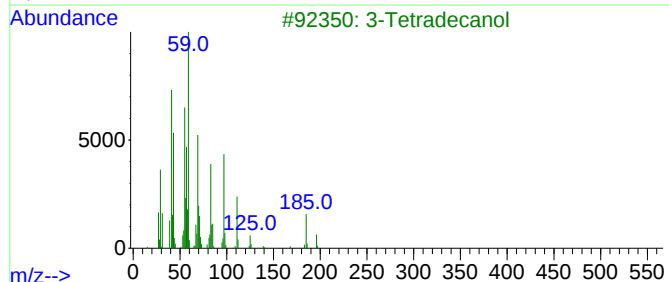
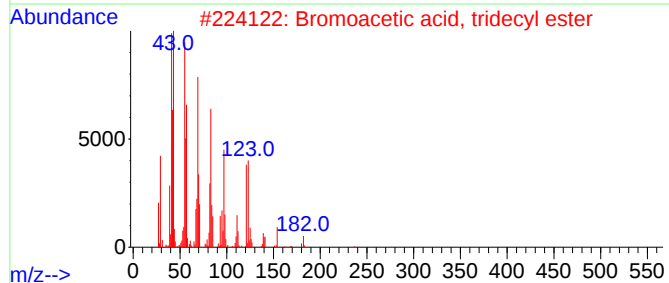
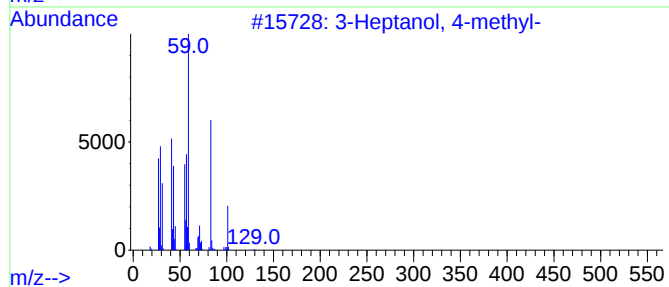
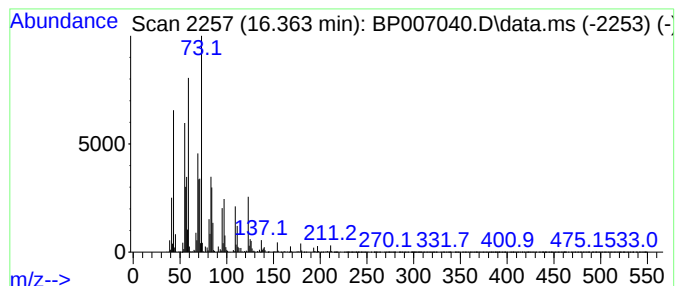
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown16.363 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.363	5.27 ng	1080740	Phenanthrene-d10	17.281

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	30
2		Bromoacetic acid, tridecyl ester	320	C15H29BrO2	1000281-85-0	27
3		3-Tetradecanol	214	C14H30O	001653-32-3	27
4		Hexylene glycol	118	C6H14O2	000107-41-5	22
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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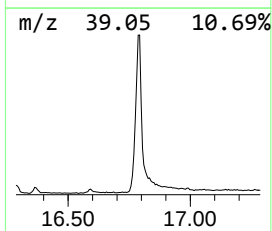
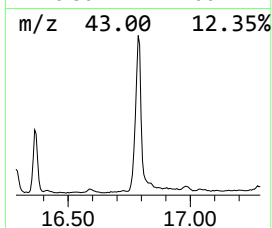
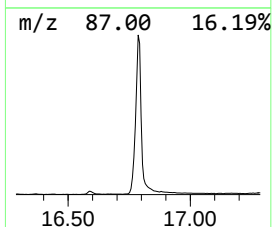
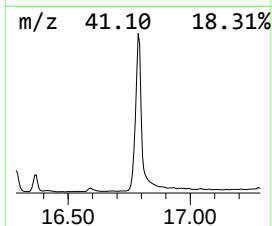
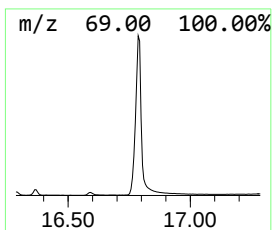
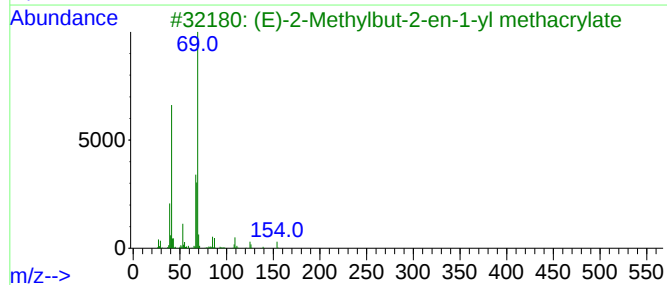
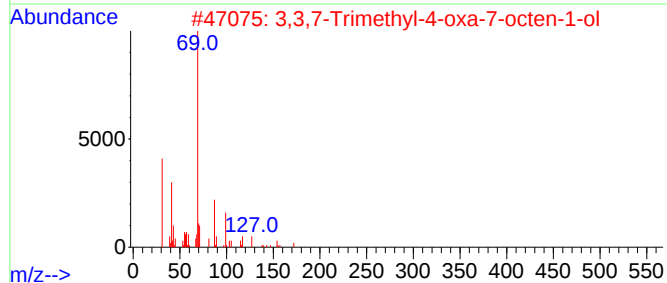
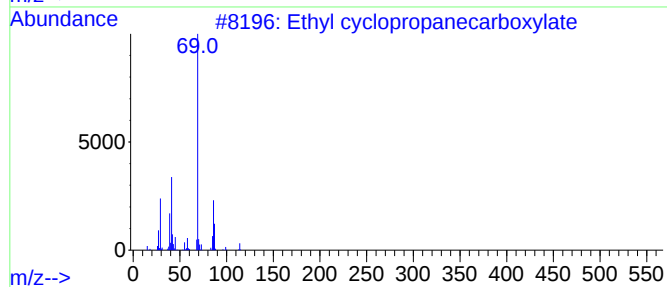
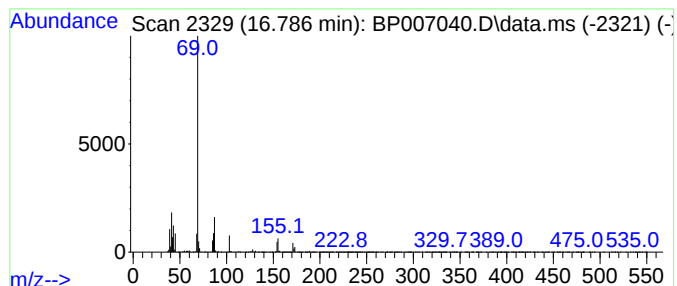
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown16.786 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.786	27.74 ng	5692790	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
2			3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	39
3			(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	38
4			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
5			1,6-Hexanediol dimethacrylate	254	C14H22O4	006606-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
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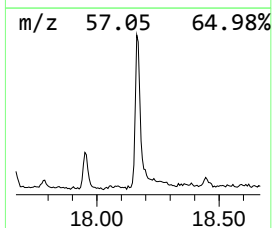
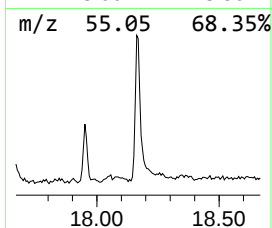
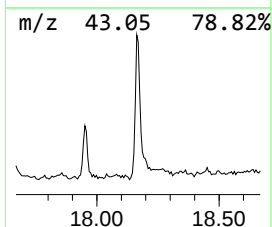
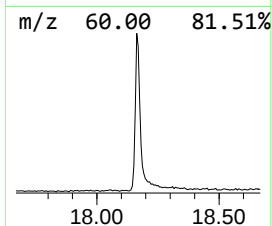
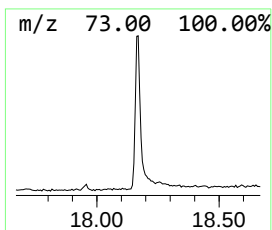
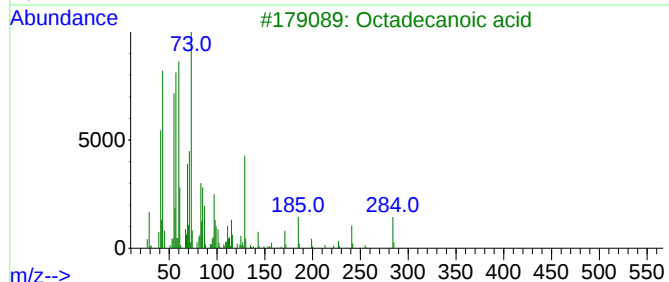
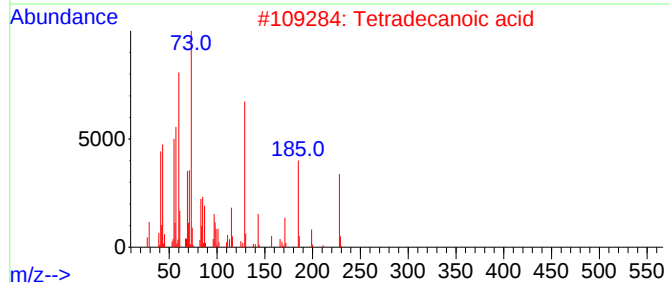
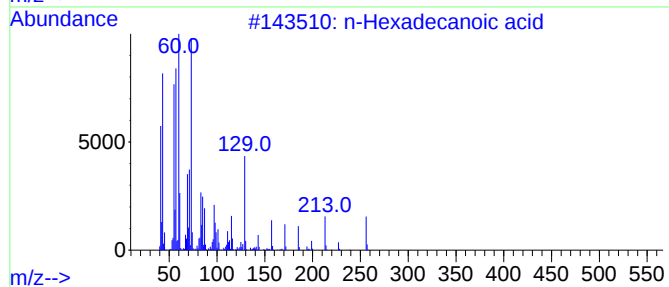
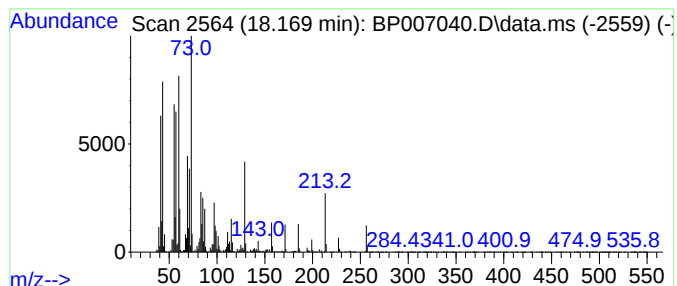
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.169	4.38 ng	898442	Phenanthrene-d10		17.281	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
3	Octadecanoic acid		284	C18H36O2	000057-11-4	90
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	Tridecanoic acid		214	C13H26O2	000638-53-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
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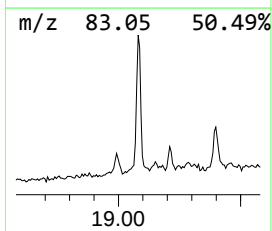
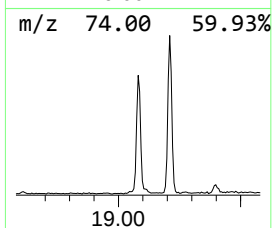
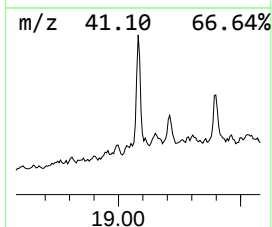
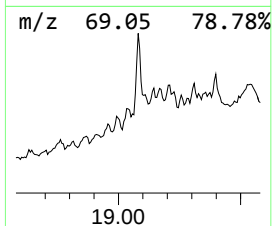
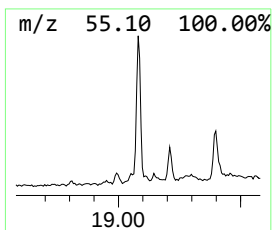
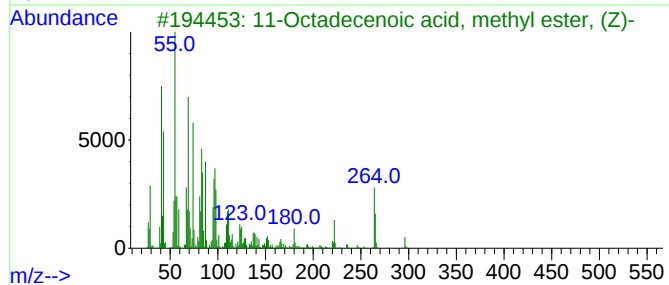
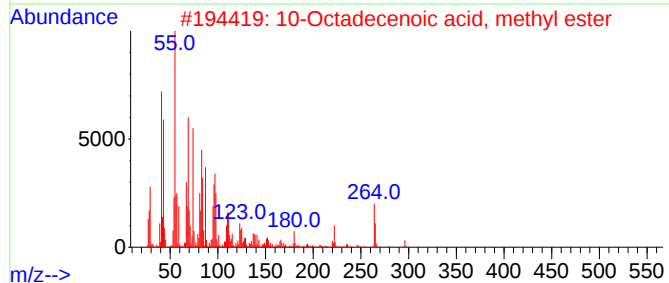
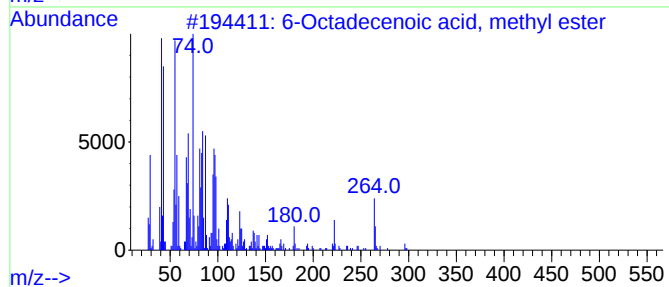
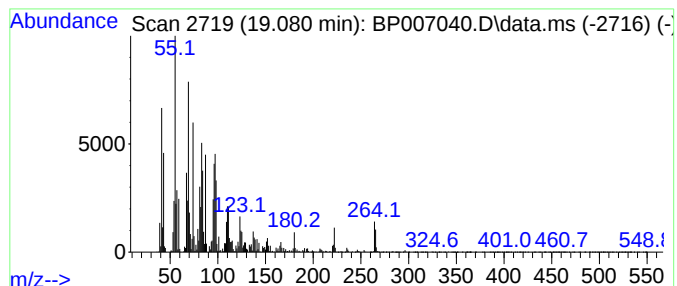
Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 6-Octadecenoic acid, methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.080	4.48 ng	918505	Phenanthrene-d10	17.281	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

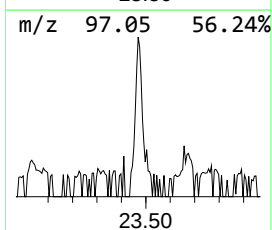
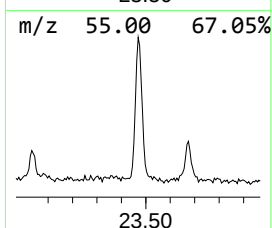
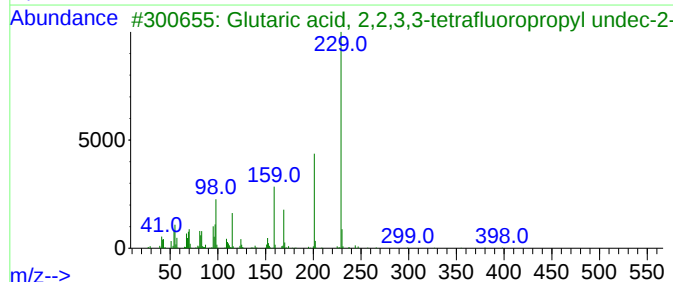
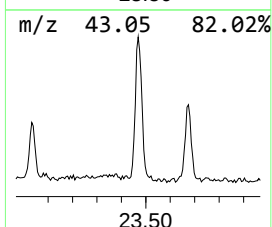
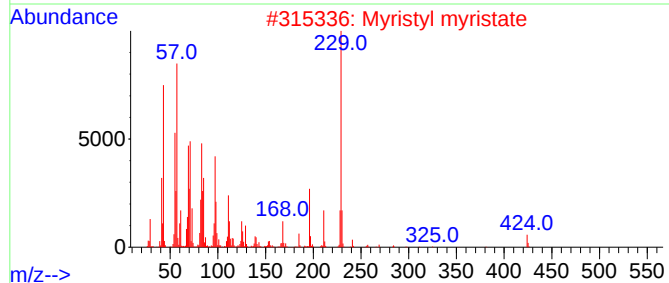
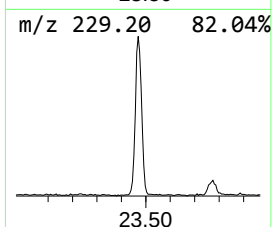
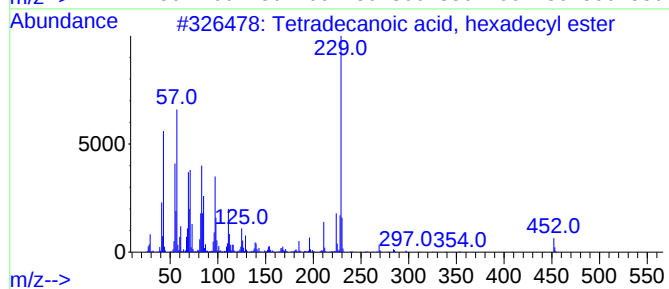
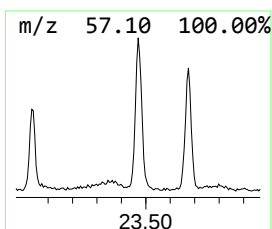
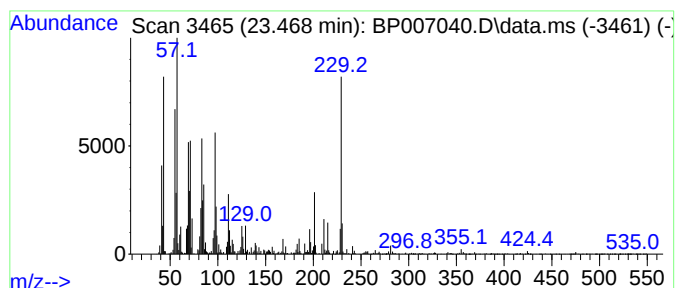
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Tetradecanoic acid, hexadec... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.468	3.19 ng	778736	Perylene-d12	23.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	74
2			Myristyl myristate	424	C28H56O2	003234-85-3	72
3			Glutaric acid, 2,2,3,3-tetraflu...	398	C19H30F4O4	1000394-01-1	35
4			Pyrimidine-4-ol, 2,6-diamino-5-b...	229	C11H11N5O	025477-74-1	27
5			Glutaric acid, 2,2,3,3-tetraflu...	368	C17H24F4O4	1000393-94-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007040.D
Acq On : 17 Sep 2021 23:02
Operator : CG/JU
Sample : M3791-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

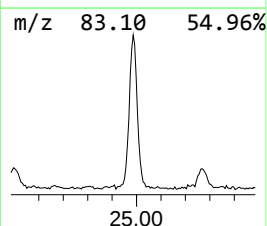
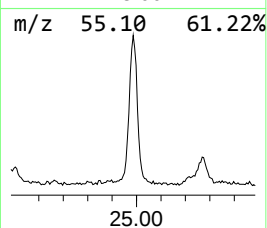
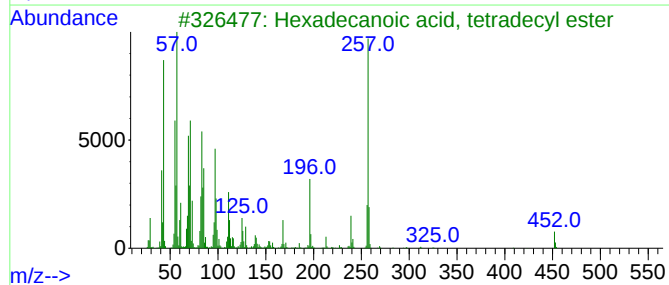
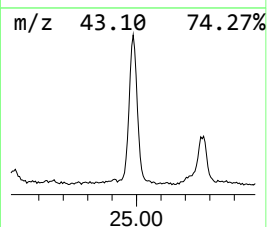
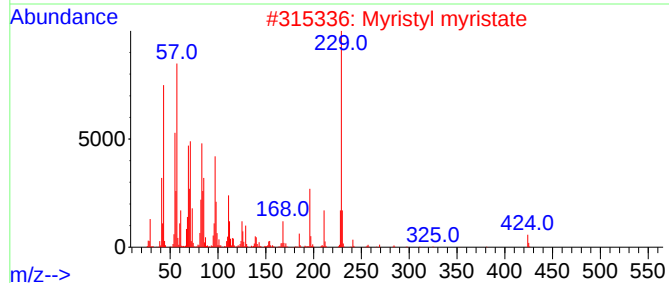
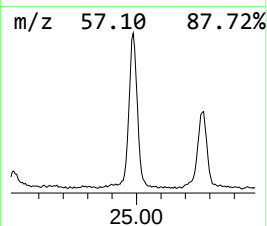
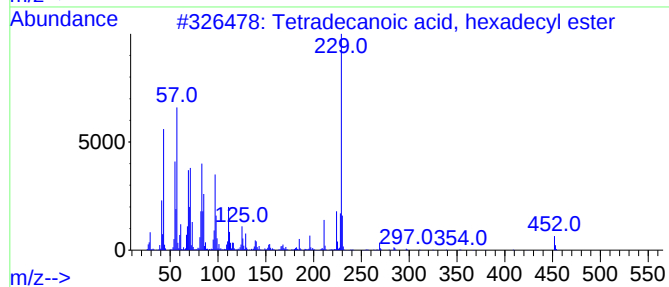
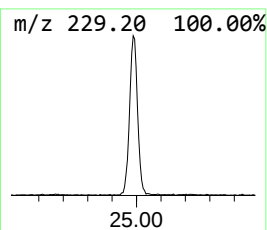
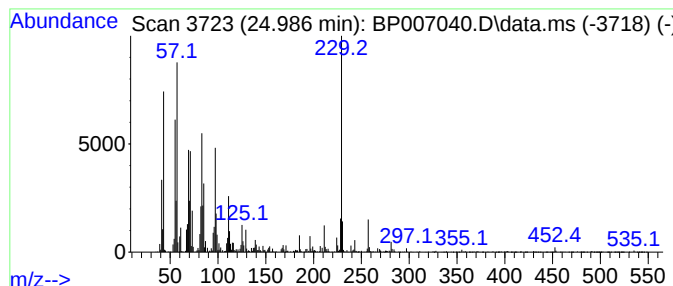
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Myristyl myristate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.986	4.96 ng	1209110	Perylene-d12	23.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	94
2			Myristyl myristate	424	C28H56O2	003234-85-3	68
3			Hexadecanoic acid, tetradecyl ester	452	C30H60O2	004536-26-9	64
4			Hexadecanoic acid, octadecyl ester	509	C34H68O2	002598-99-4	52
5			Glutaric acid, 1-cyclopentylethy...	342	C15H22F4O4	1000405-45-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
 Data File : BP007040.D
 Acq On : 17 Sep 2021 23:02
 Operator : CG/JU
 Sample : M3791-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.316	4.316	2.9	ng	287570	1	7.905	1977760	20.0
Crotonic acid	4.669	6.4	ng	634164	1	7.905	1977760	20.0
Butane, 2,3-dim...	4.728	3.6	ng	357578	1	7.905	1977760	20.0
Butanoic acid, ...	4.799	7.9	ng	779921	1	7.905	1977760	20.0
2-Pentanone, 4-...	5.022	3.3	ng	326588	1	7.905	1977760	20.0
Cyclohexanecarb...	9.393	19.1	ng	2607060	2	10.704	2722110	20.0
Phenol, 3-ethyl-	10.152	25.1	ng	3423300	2	10.704	2722110	20.0
Ethanol, 2-(2-b...	10.487	20.9	ng	2849650	2	10.704	2722110	20.0
Benzeneacetic acid	11.246	5.1	ng	692606	2	10.704	2722110	20.0
unknown12.398	12.398	41.1	ng	5595540	2	10.704	2722110	20.0
Hydrocinnamic acid	12.557	54.6	ng	7427220	2	10.704	2722110	20.0
2,4,7,9-Tetrame...	13.440	3.2	ng	593589	3	14.534	3670500	20.0
3-Octanol, 2,2-...	13.493	2.2	ng	410107	3	14.534	3670500	20.0
unknown16.286	16.286	5.3	ng	1087490	4	17.281	4104880	20.0
unknown16.363	16.363	5.3	ng	1080740	4	17.281	4104880	20.0
unknown16.786	16.786	27.7	ng	5692790	4	17.281	4104880	20.0
n-Hexadecanoic ...	18.169	4.4	ng	898442	4	17.281	4104880	20.0
6-Octadecenoic ...	19.080	4.5	ng	918505	4	17.281	4104880	20.0
Tetradecanoic a...	23.468	3.2	ng	778736	6	23.768	4875200	20.0
Myristyl myristate	24.986	5.0	ng	1209110	6	23.768	4875200	20.0