

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
 Data File : BF136099.D
 Acq On : 02 Nov 2023 16:59
 Operator : CG\JU
 Sample : 05005-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-2(5-10)

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_F\Methods\8270-BF103023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	414407	415439	13.37%	1.671%
2	2.322	35	40	44	rVB	30035	42260	1.36%	0.170%
3	2.946	138	146	154	rVB	47915	81033	2.61%	0.326%
4	3.375	212	219	234	rBV2	28654	77010	2.48%	0.310%
5	4.440	393	400	403	rBV	1194105	1407645	45.29%	5.663%
6	5.057	498	505	518	rVB	1448816	2098046	67.51%	8.441%
7	5.457	567	573	576	rBV	2709310	2755842	88.67%	11.087%
8	5.840	635	638	642	rVB	121629	94806	3.05%	0.381%
9	6.451	737	742	745	rBV	2444677	2714164	87.33%	10.919%
10	6.646	772	775	788	rVB	45924	64138	2.06%	0.258%
11	6.816	801	804	808	rBV	823198	663487	21.35%	2.669%
12	7.381	895	900	903	rBV	2002888	1774079	57.08%	7.137%
13	8.098	1018	1022	1025	rBV	1207767	900033	28.96%	3.621%
14	9.181	1202	1206	1209	rVB	3845233	3107897	100.00%	12.503%
15	9.298	1223	1226	1233	rVB	118492	114060	3.67%	0.459%
16	9.857	1317	1321	1324	rBV	1245497	953811	30.69%	3.837%
17	10.651	1451	1456	1459	rBV	1969415	1867965	60.10%	7.515%
18	10.786	1474	1479	1482	rBV	92493	96559	3.11%	0.388%
19	11.251	1555	1558	1562	rVB	174730	167928	5.40%	0.676%
20	11.345	1571	1574	1578	rBV	914852	850360	27.36%	3.421%
21	11.604	1615	1618	1621	rBV	92192	91138	2.93%	0.367%
22	11.757	1641	1644	1648	rVB4	42787	57650	1.85%	0.232%
23	11.886	1662	1666	1670	rBV	317346	319202	10.27%	1.284%
24	12.128	1704	1707	1709	rBV2	44087	46043	1.48%	0.185%
25	12.345	1742	1744	1749	rVB	120408	135235	4.35%	0.544%
26	12.569	1778	1782	1785	rBV2	157174	189084	6.08%	0.761%
27	12.680	1798	1801	1803	rBV	138762	117790	3.79%	0.474%
28	12.798	1819	1821	1824	rVB	123479	86586	2.79%	0.348%
29	12.951	1843	1847	1850	rBV	2626079	2286224	73.56%	9.198%
30	14.004	2021	2026	2029	rBV	752590	699092	22.49%	2.813%
31	15.051	2201	2204	2207	rBV	26243	37135	1.19%	0.149%
32	15.163	2220	2223	2227	rVB	34597	41350	1.33%	0.166%
33	15.492	2274	2279	2284	rBV	428750	503454	16.20%	2.025%

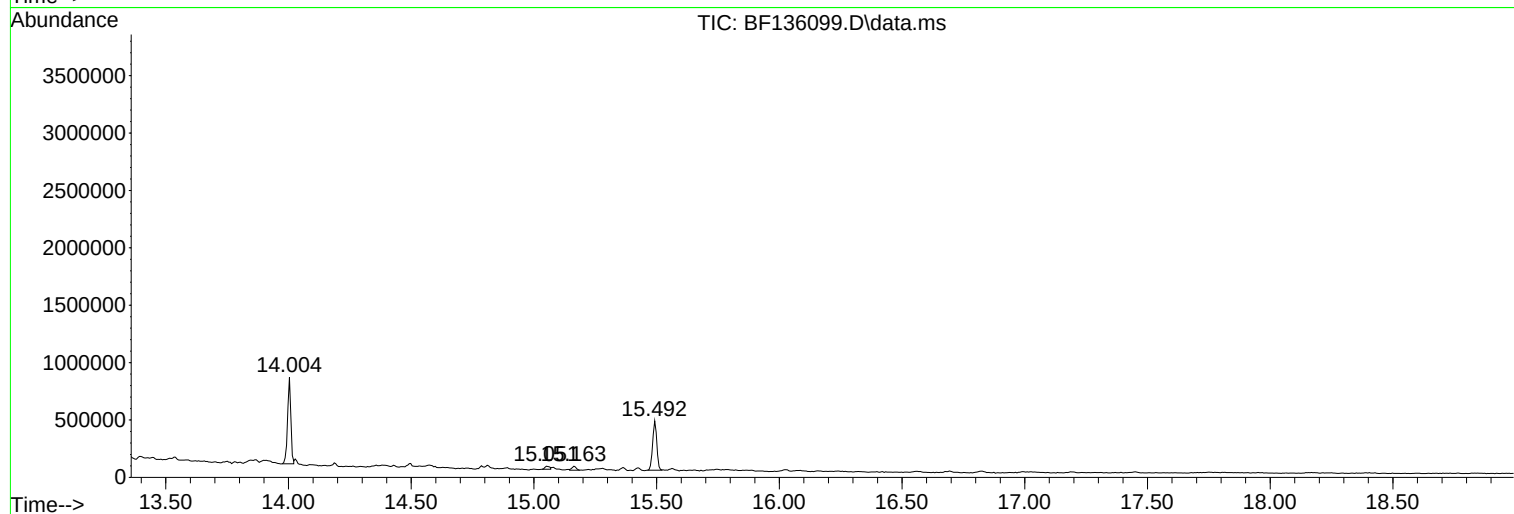
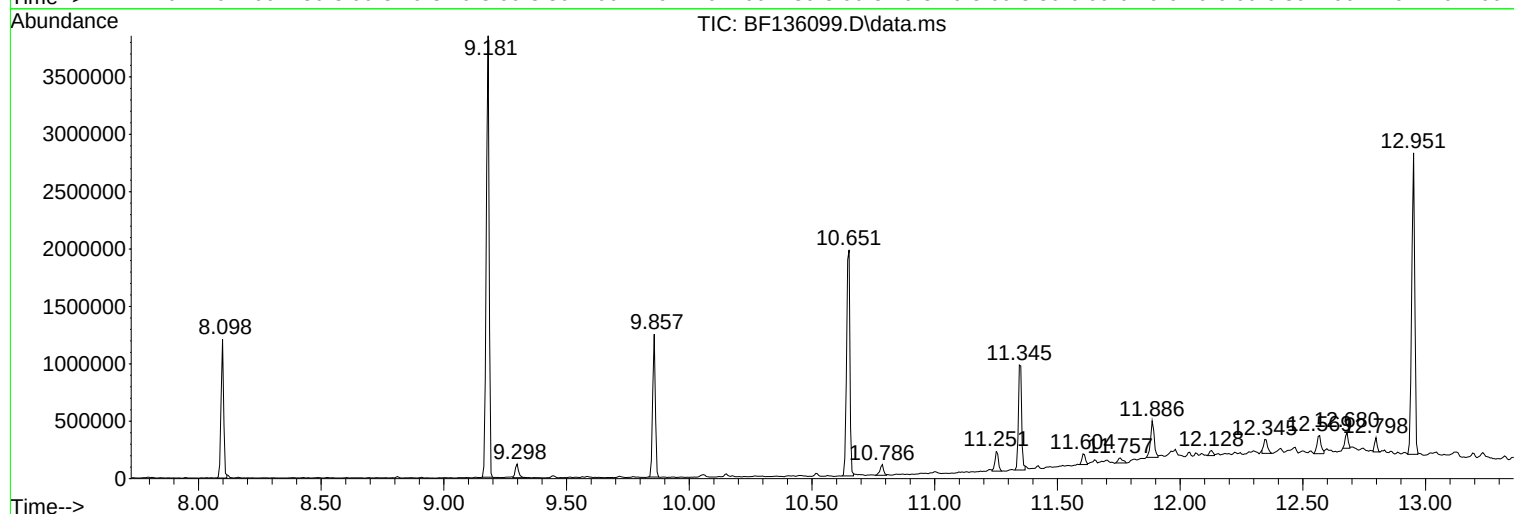
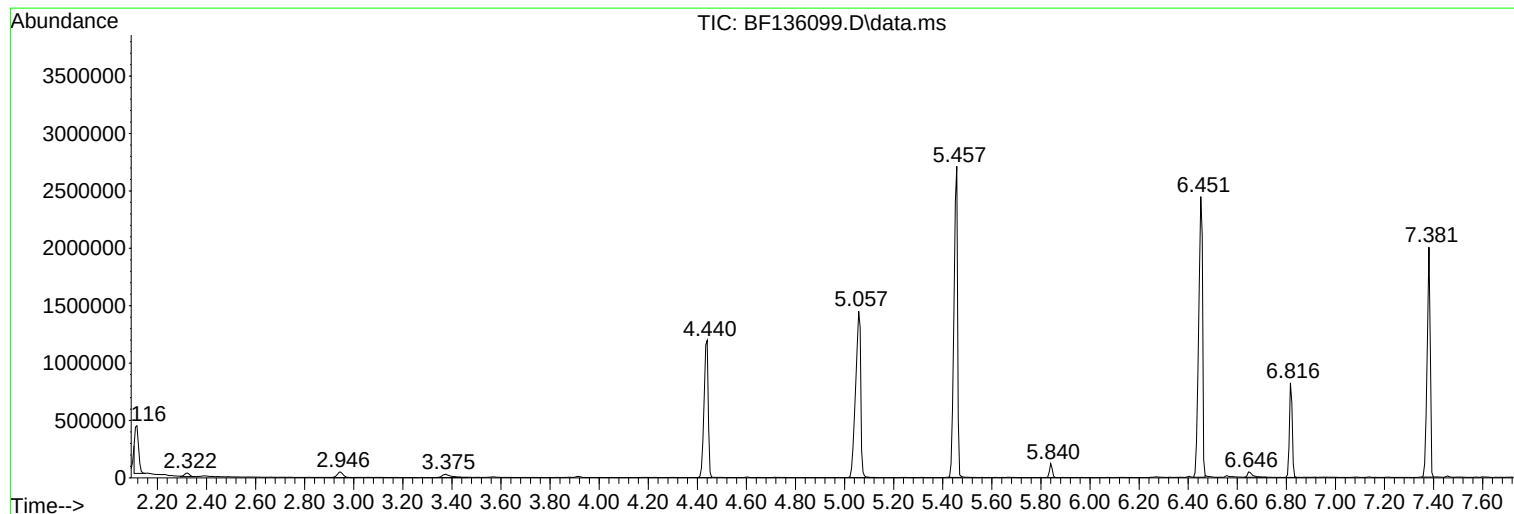
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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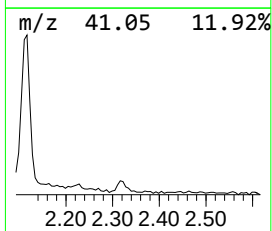
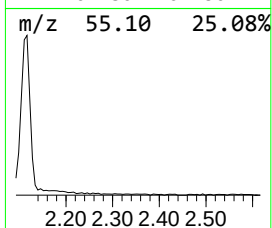
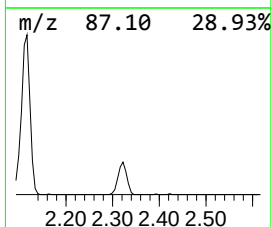
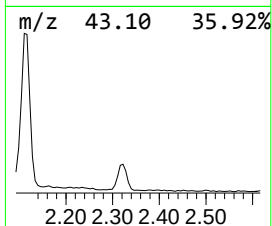
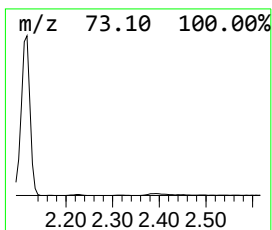
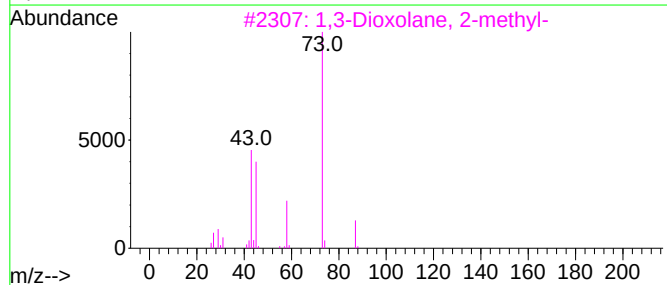
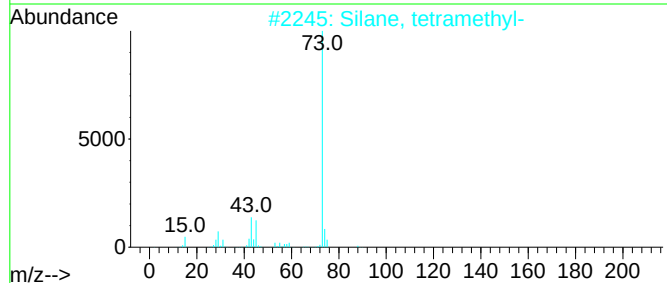
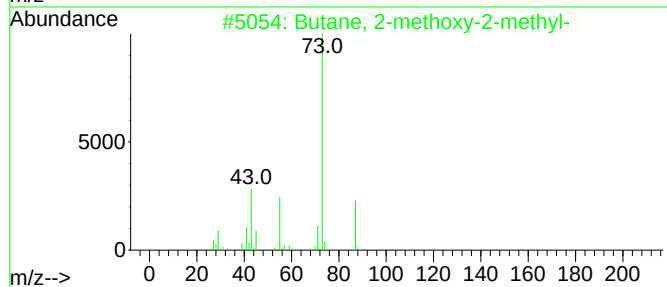
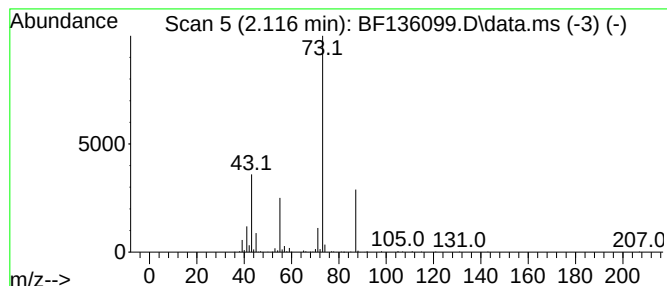
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	12.52 ng	415439	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	23



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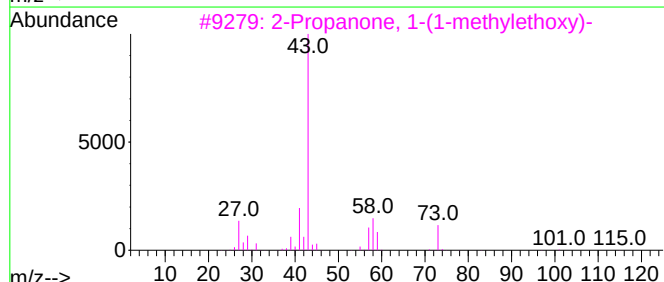
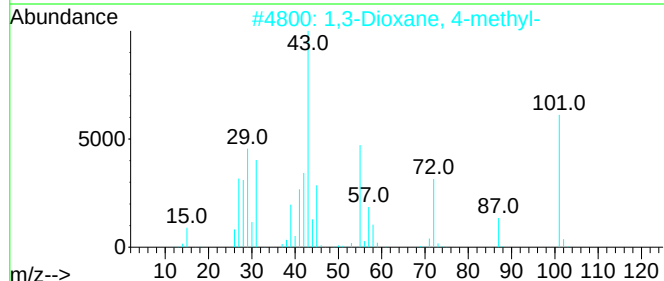
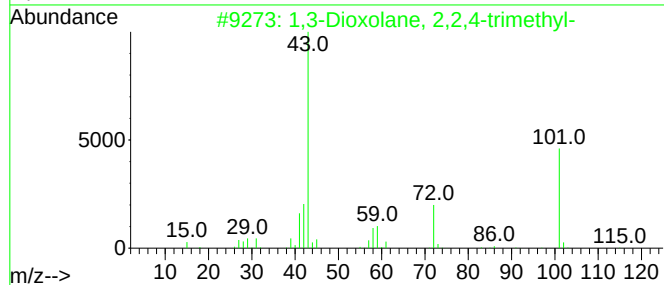
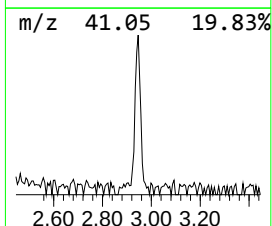
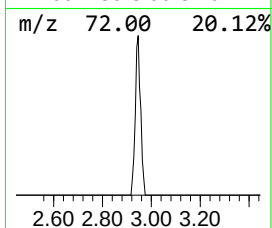
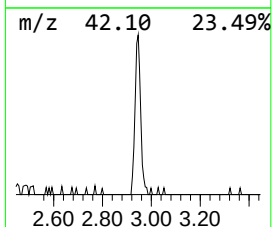
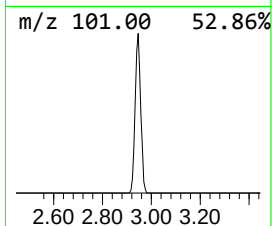
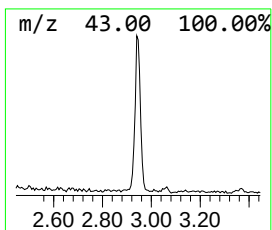
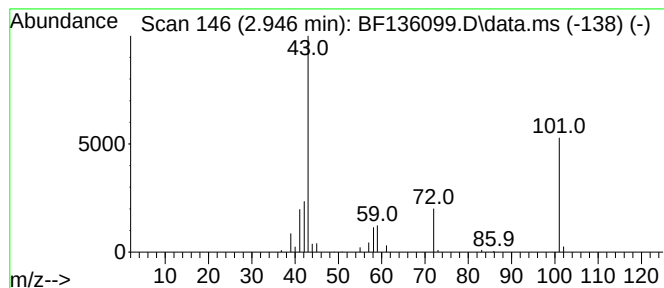
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.946	2.44 ng	81033	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	59
3		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10
4		2-Butanone	72	C4H8O	000078-93-3	9
5		2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	9



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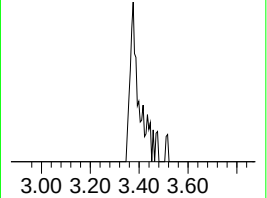
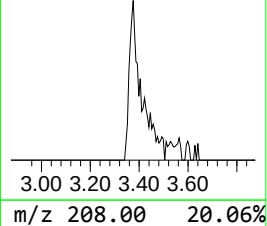
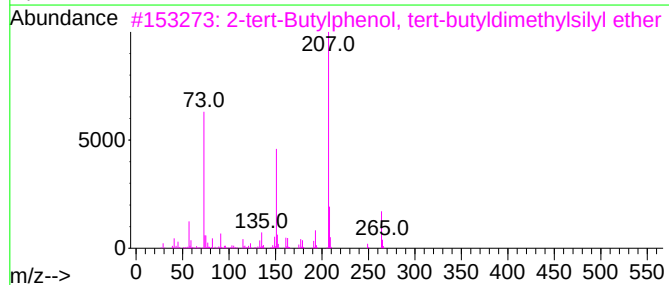
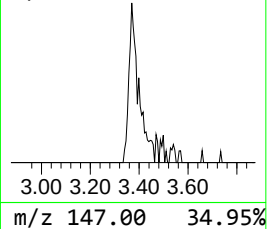
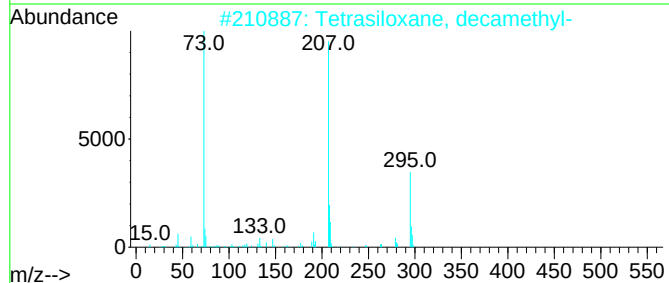
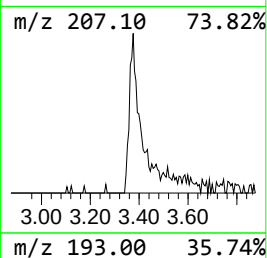
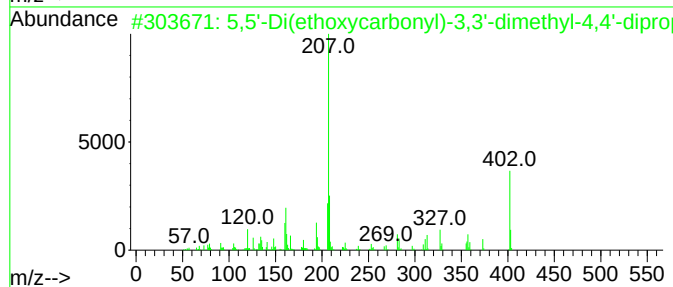
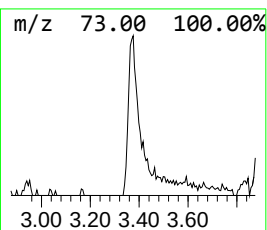
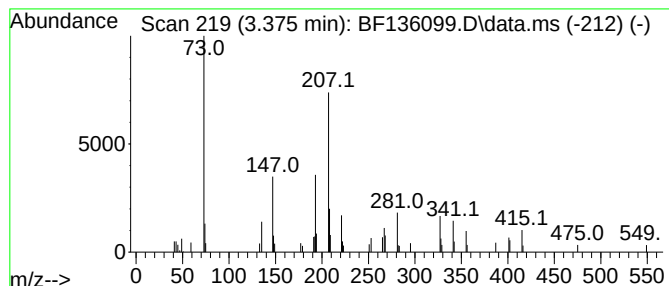
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 5,5'-Di(ethoxycarbonyl)-3,3... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	2.32 ng	77010	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	59	
2	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	47	
3	2-tert-Butylphenol, tert-butyldi...	264	C16H28OSi	860465-21-0	47	
4	2,4,6-Cycloheptatrien-1-one, 3,5...	250	C13H22OSi2	1000161-21-8	47	
5	2-Propanesulfonamide, N-[2-(4'-c...	342	C19H22N2O2S	211311-95-4	43	



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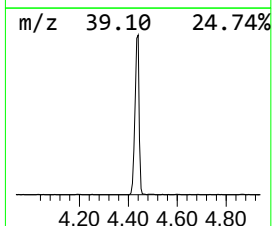
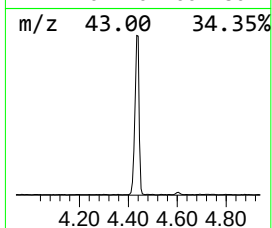
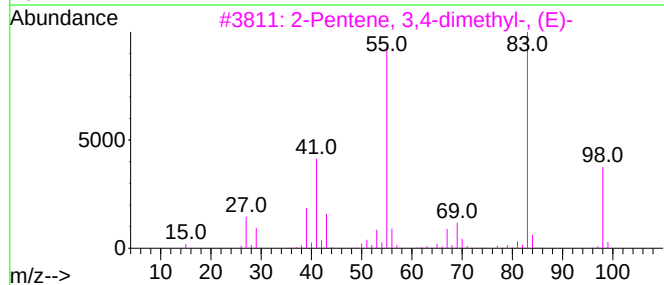
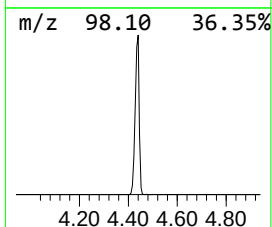
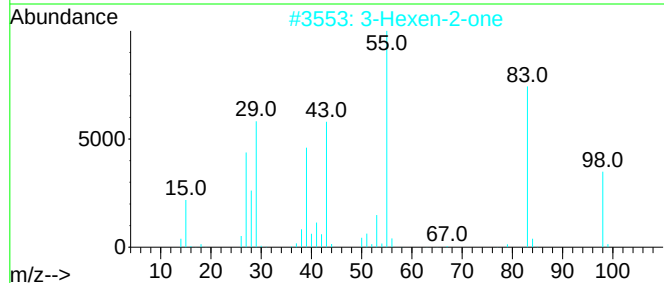
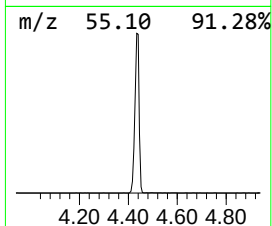
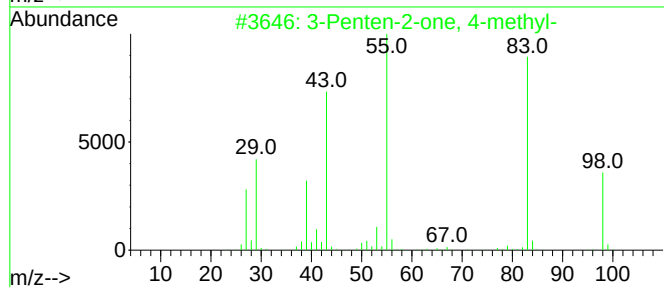
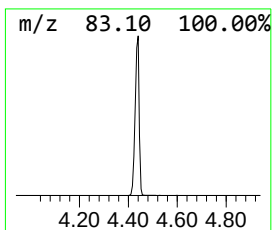
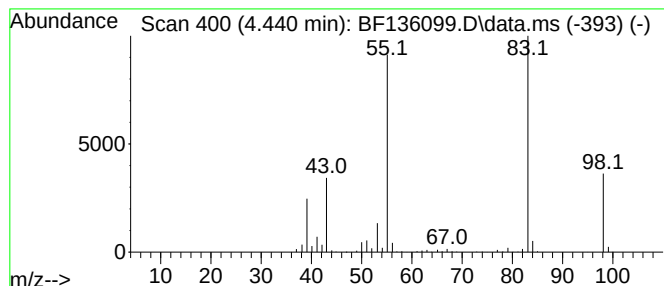
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Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	42.43 ng	1407650	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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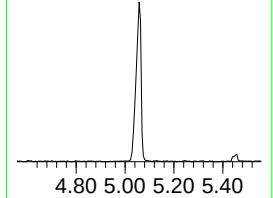
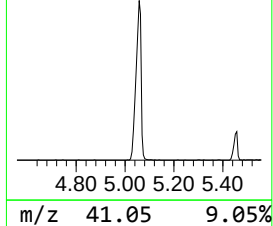
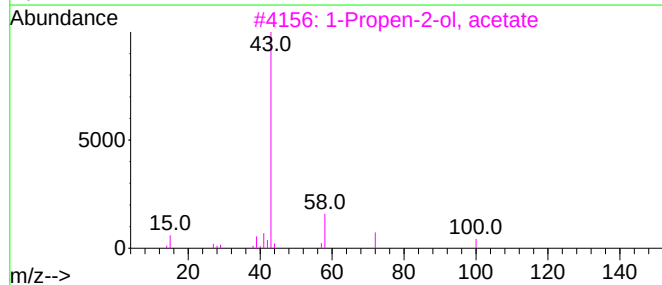
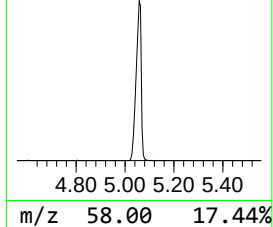
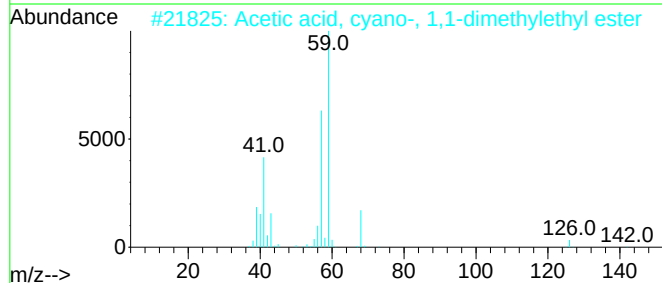
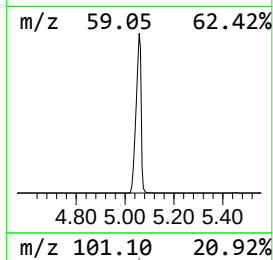
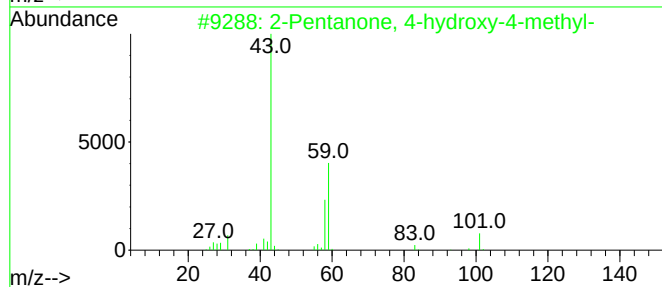
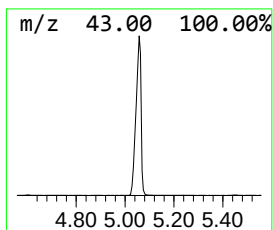
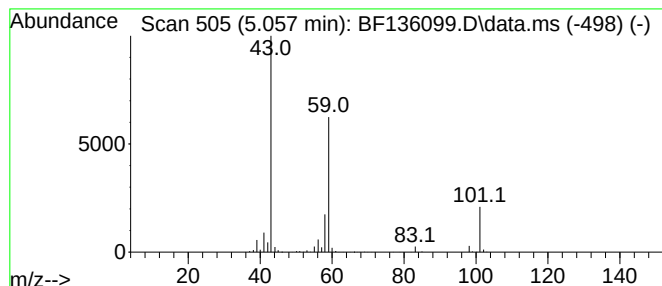
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.057	63.24 ng	2098050	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9



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ClientSampleId :
N-2(5-10)

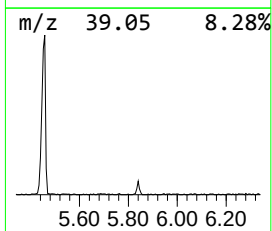
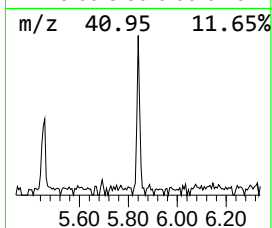
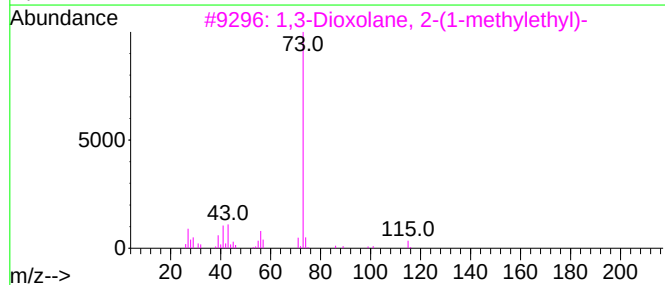
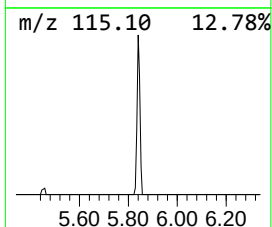
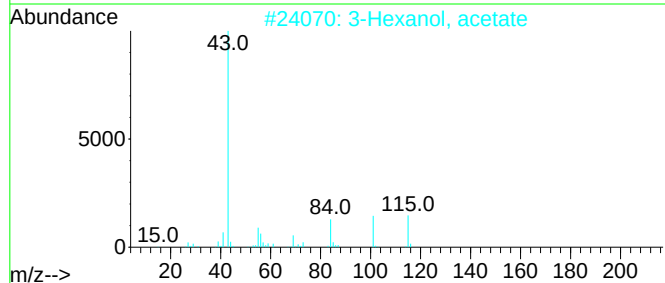
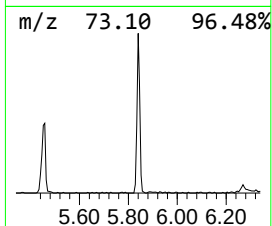
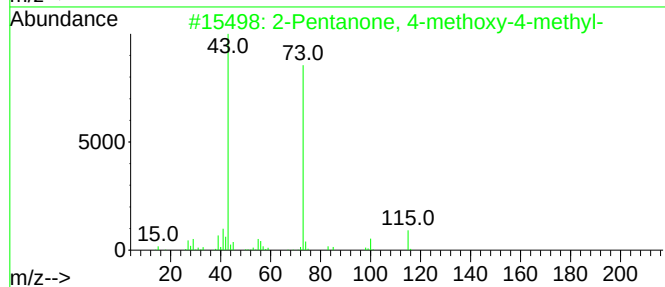
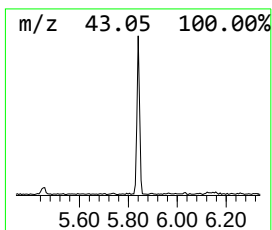
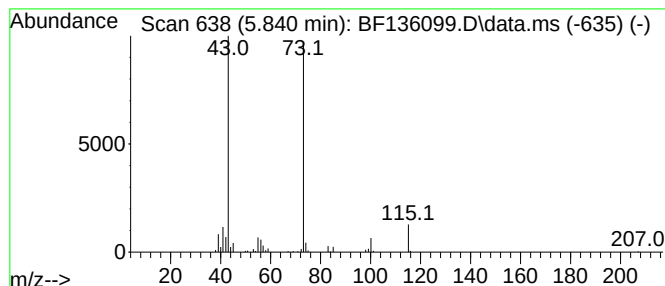
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.840	2.86 ng	94806	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		3-Hexanol, acetate	144	C8H16O2	040780-64-1	23
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	22
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	22
5		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
Operator : CG\JU
Sample : 05005-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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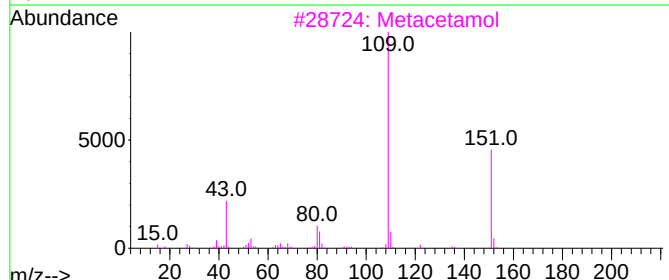
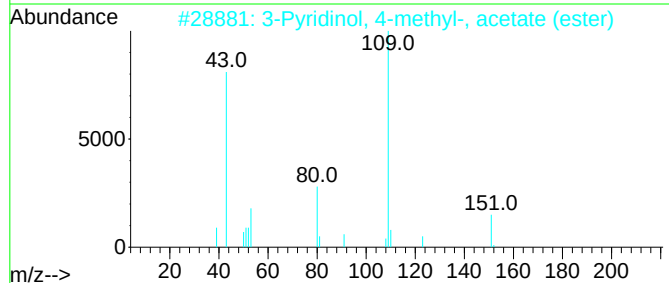
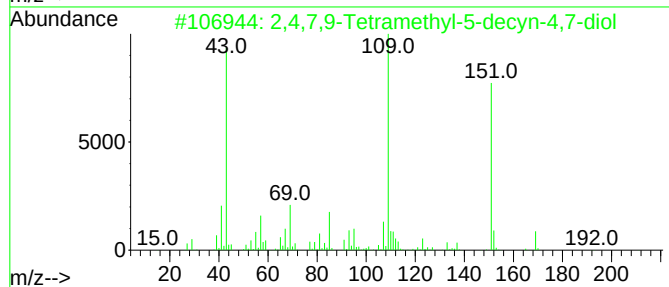
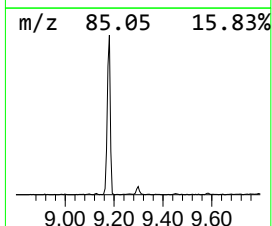
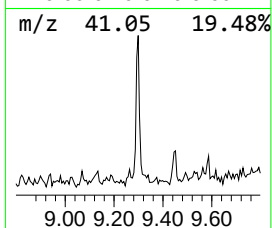
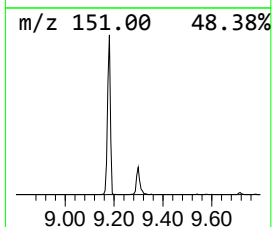
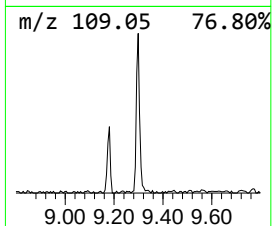
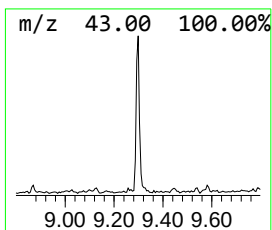
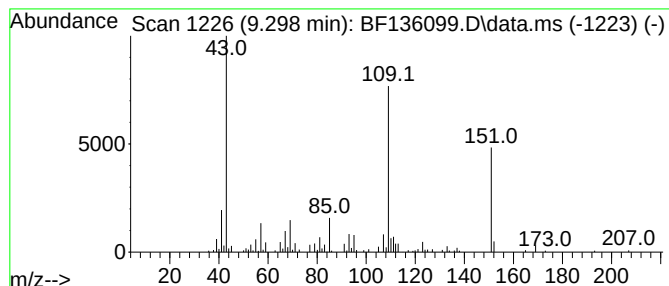
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	2.39 ng	114060	Acenaphthene-d10	9.857

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	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	64	
3	Metacetamol	151	C8H9NO2	000621-42-1	64	
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
N-2(5-10)

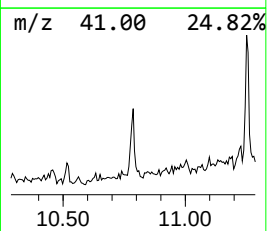
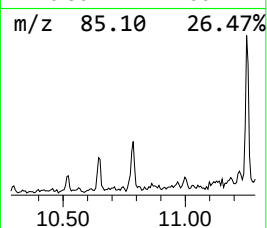
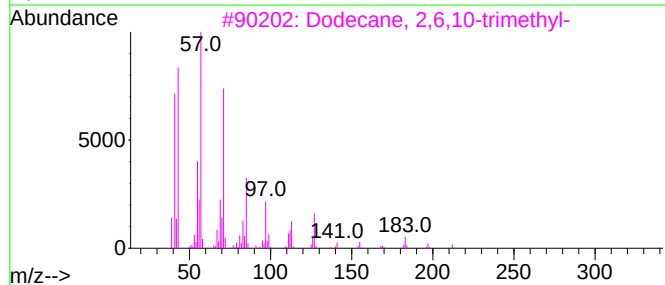
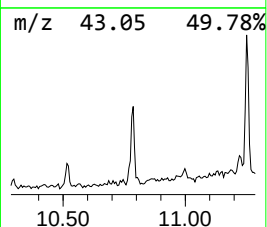
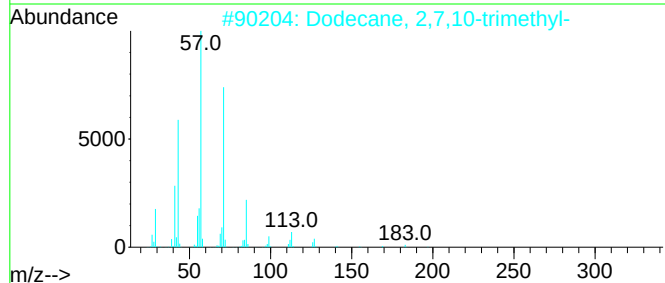
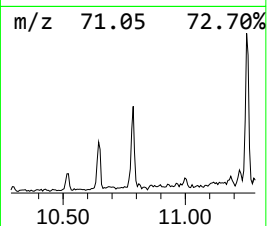
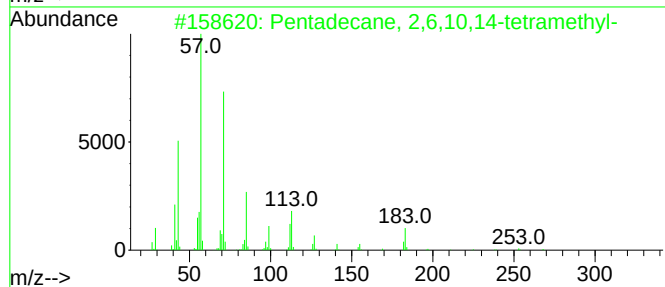
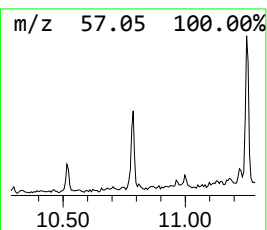
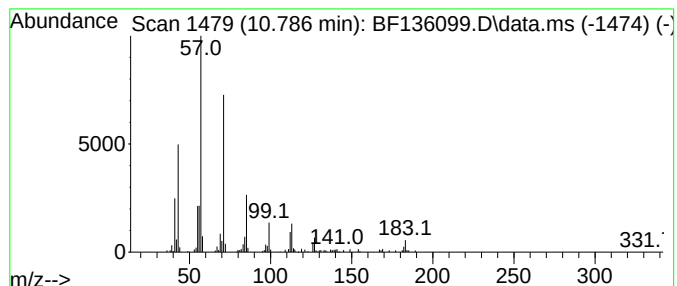
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 2,6,10,14-tetr... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	2.27 ng	96559	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78
4			Tridecane, 5-propyl-	226	C16H34	055045-11-9	72
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
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ALS Vial : 10 Sample Multiplier: 1

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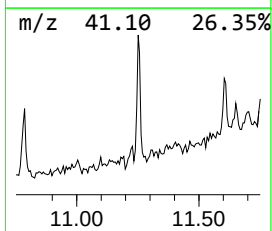
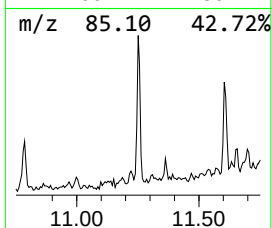
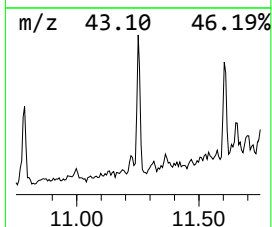
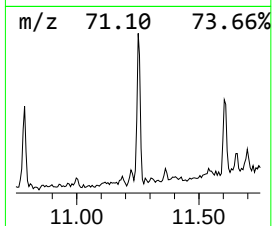
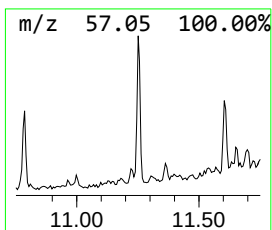
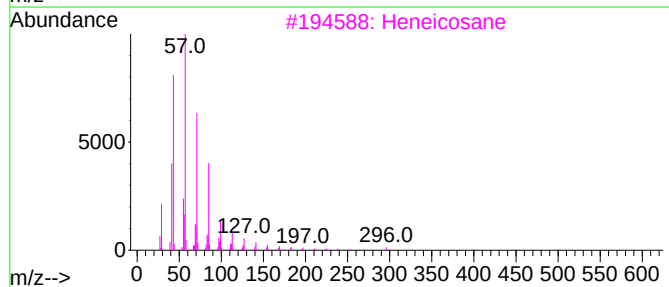
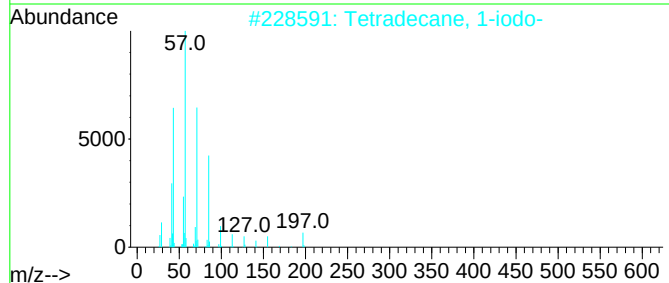
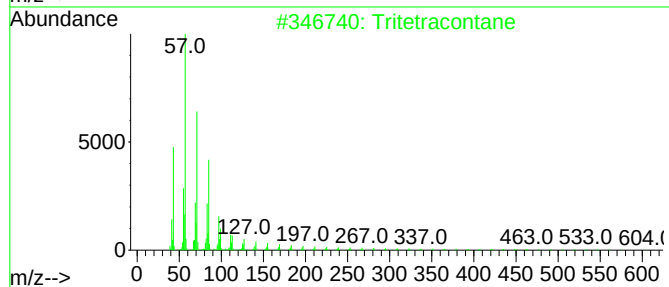
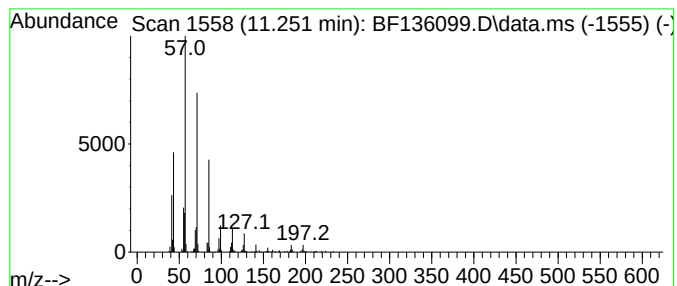
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tritetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	3.95 ng	167928	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	90
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
5			Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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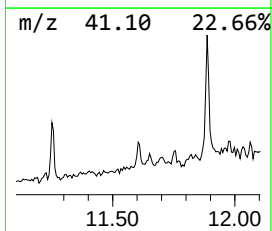
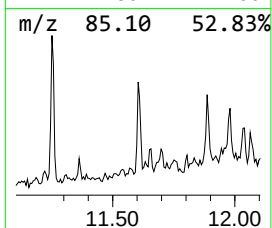
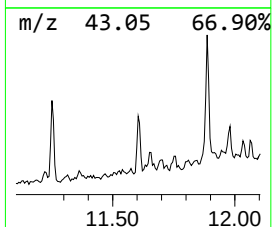
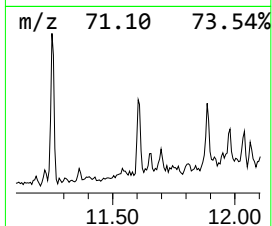
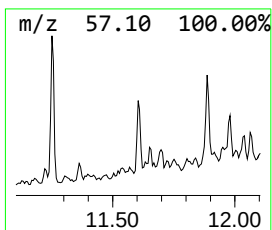
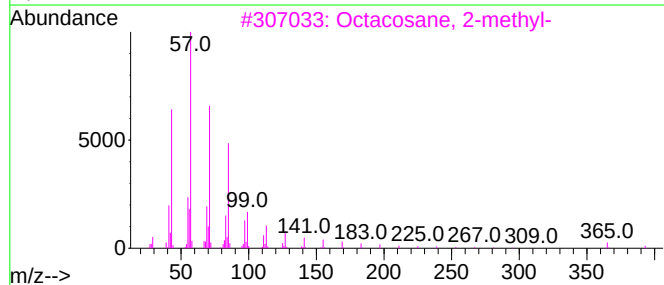
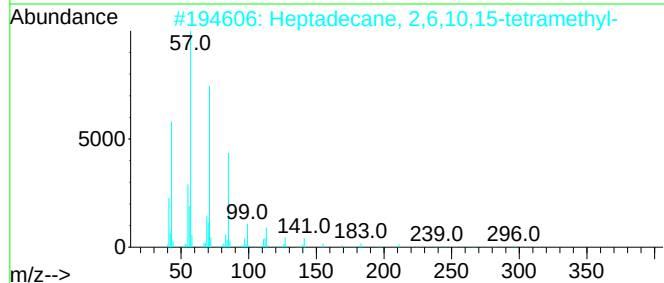
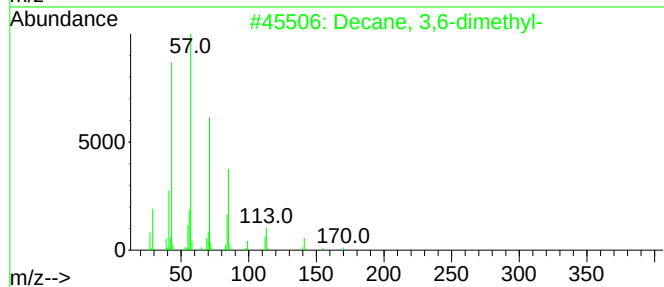
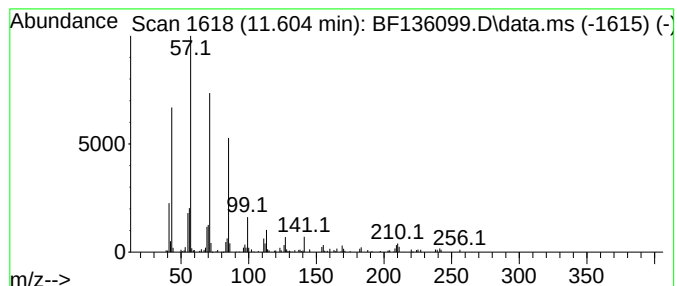
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Decane, 3,6-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	2.14 ng	91138	Phenanthrene-d10	11.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	87
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4		Heneicosane	296	C21H44	000629-94-7	86
5		Dodecane	170	C12H26	000112-40-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
Operator : CG\JU
Sample : 05005-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
N-2(5-10)

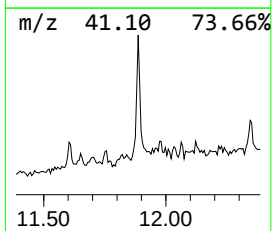
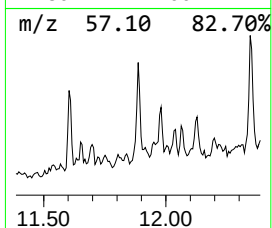
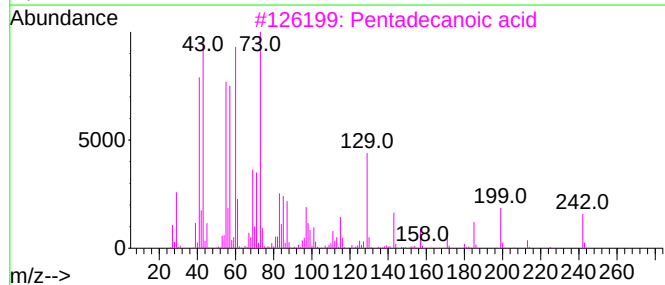
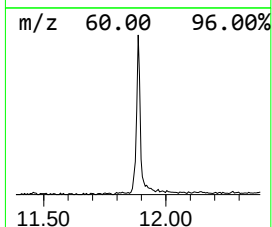
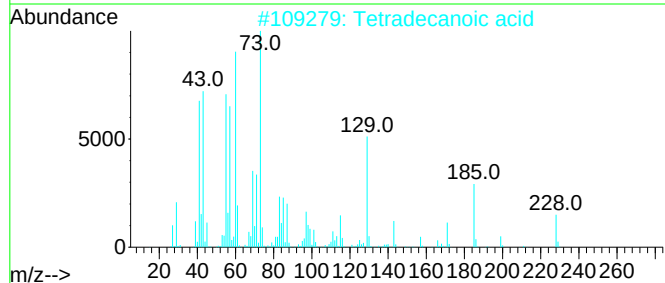
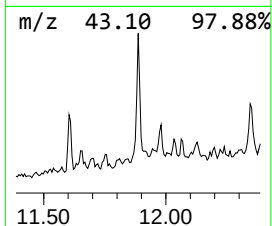
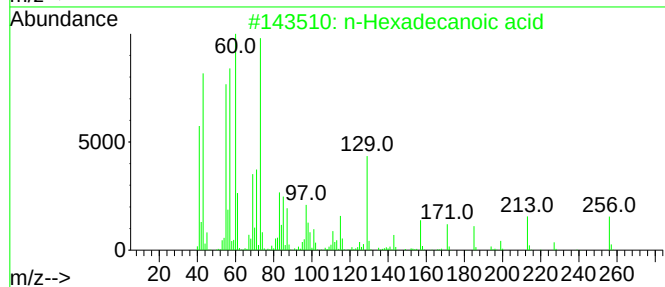
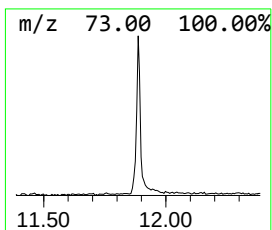
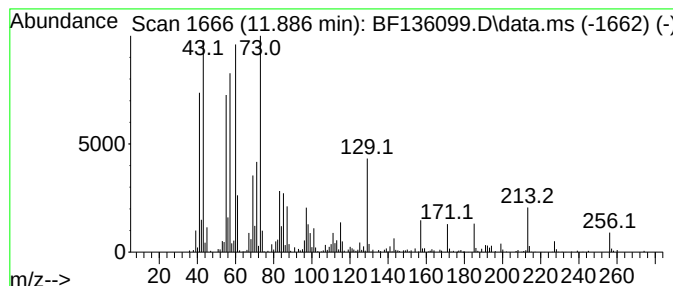
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	7.51 ng	319202	Phenanthrene-d10	11.351

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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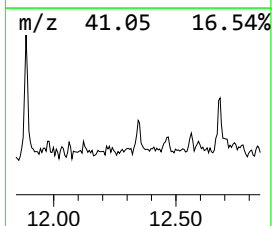
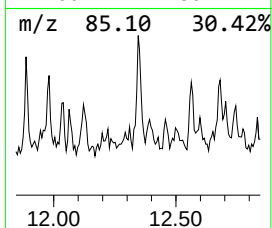
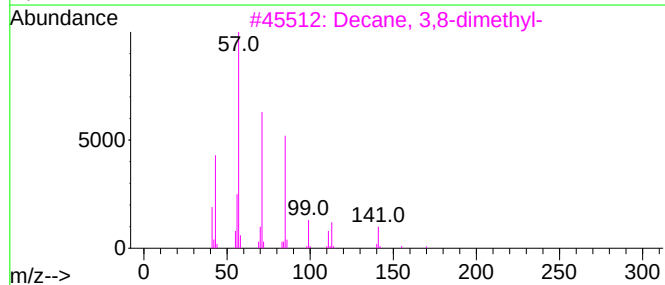
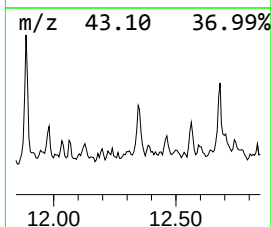
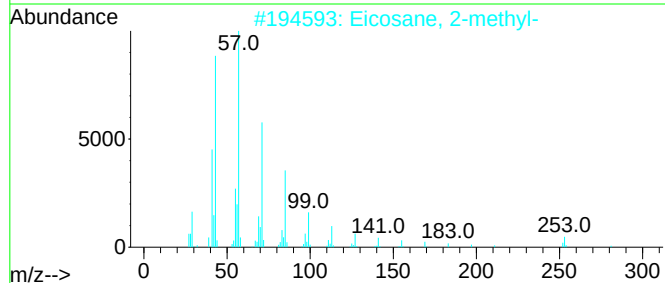
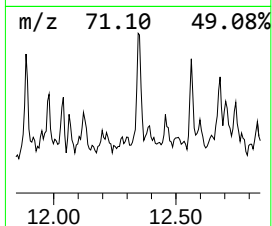
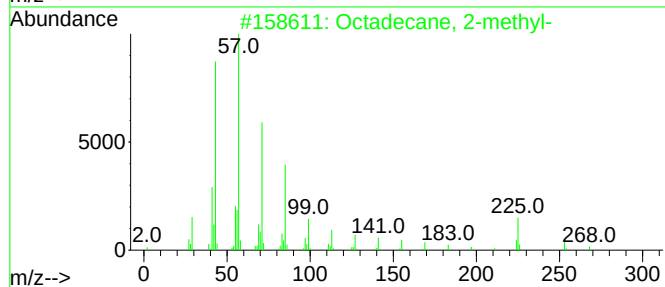
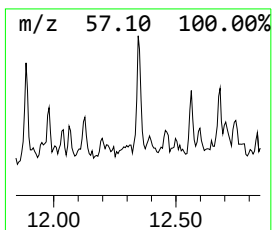
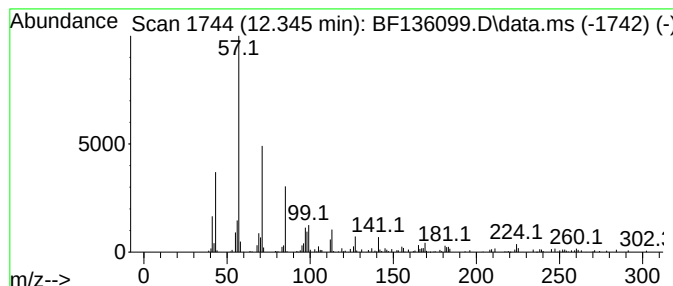
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	3.18 ng	135235	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
2			Eicosane, 2-methyl-	296	C21H44	001560-84-5	72
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	70
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	68
5			triacontane	422	C30H62	000638-68-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
Operator : CG\JU
Sample : 05005-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

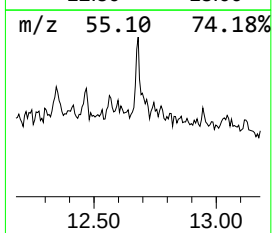
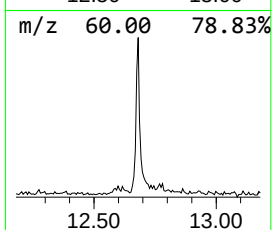
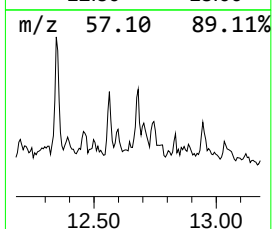
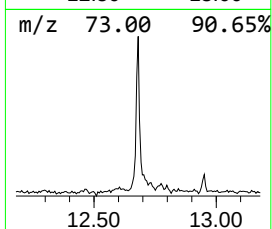
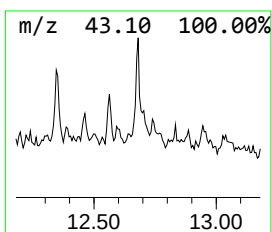
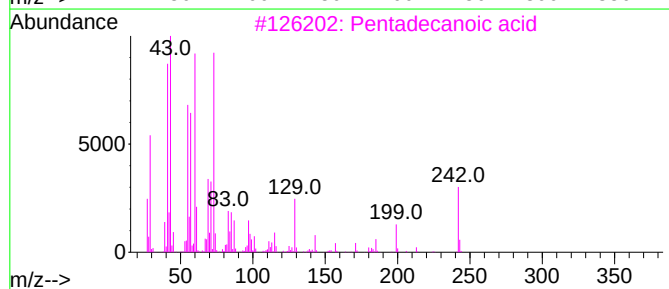
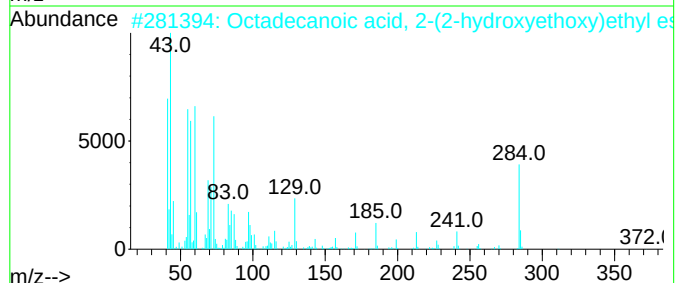
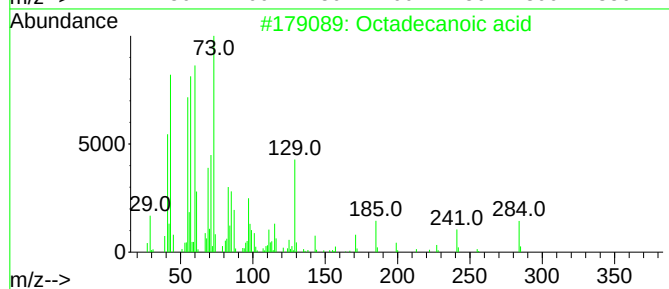
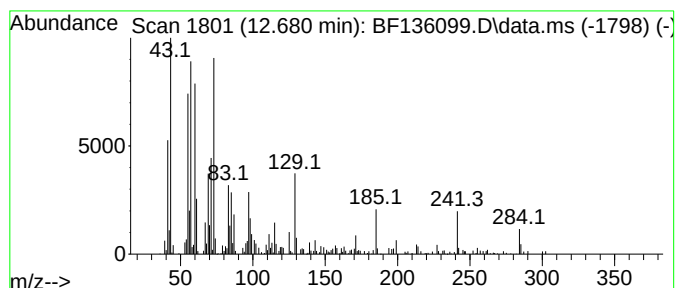
Instrument :
BNA_F
ClientSampleId :
N-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.680	3.37 ng	117790	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136099.D
Acq On : 02 Nov 2023 16:59
Operator : CG\JU
Sample : 05005-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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
Butane, 2-metho...	2.116	12.5	ng	415439	1	6.816	663487	20.0
1,3-Dioxolane, ...	2.946	2.4	ng	81033	1	6.816	663487	20.0
5,5'-Di(ethoxyc...	3.375	2.3	ng	77010	1	6.816	663487	20.0
3-Penten-2-one,...	4.440	42.4	ng	1407650	1	6.816	663487	20.0
2-Pentanone, 4-...	5.057	63.2	ng	2098050	1	6.816	663487	20.0
2-Pentanone, 4-...	5.840	2.9	ng	94806	1	6.816	663487	20.0
2,4,7,9-Tetrame...	9.298	2.4	ng	114060	3	9.857	953811	20.0
Pentadecane, 2,...	10.786	2.3	ng	96559	4	11.351	850360	20.0
Tritetracontane	11.251	4.0	ng	167928	4	11.351	850360	20.0
Decane, 3,6-dim...	11.604	2.1	ng	91138	4	11.351	850360	20.0
n-Hexadecanoic ...	11.886	7.5	ng	319202	4	11.351	850360	20.0
Octadecane, 2-m...	12.345	3.2	ng	135235	4	11.351	850360	20.0
Octadecanoic acid	12.680	3.4	ng	117790	5	14.004	699092	20.0