

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
 Data File : BP007055.D
 Acq On : 20 Sep 2021 18:01
 Operator : CG/JU
 Sample : M3687-29
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A004145

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

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	24	29	43	rVB	218816	352349	2.23%	0.400%
2	5.016	323	328	338	rBV	784139	1123485	7.13%	1.276%
3	5.481	400	407	420	rBV	4356446	6298581	39.95%	7.152%
4	7.075	670	678	694	rBV	4033103	6531179	41.42%	7.417%
5	7.905	812	819	827	rBV	1024122	1629660	10.34%	1.851%
6	9.069	1009	1017	1032	rBV	2490757	4178724	26.50%	4.745%
7	10.487	1251	1258	1272	rBV	897143	1539119	9.76%	1.748%
8	10.704	1287	1295	1303	rBV	1307598	2210464	14.02%	2.510%
9	13.163	1706	1713	1729	rBV	6992770	10129596	64.25%	11.503%
10	14.534	1939	1946	1953	rBV	2011499	2933595	18.61%	3.331%
11	14.951	2009	2017	2031	rBV	269247	539668	3.42%	0.613%
12	16.022	2192	2199	2211	rBV	5309264	7911177	50.18%	8.984%
13	16.681	2307	2311	2322	rVB3	87859	158806	1.01%	0.180%
14	17.280	2407	2413	2425	rVB	2411547	3527163	22.37%	4.005%
15	17.951	2523	2527	2533	rBV	176135	215871	1.37%	0.245%
16	18.175	2557	2565	2593	rBV	3243628	5498540	34.87%	6.244%
17	19.286	2746	2754	2758	rBV4	218224	513822	3.26%	0.583%
18	19.398	2769	2773	2778	rBV	1878863	2549875	16.17%	2.896%
19	19.516	2788	2793	2809	rVB	757123	2380393	15.10%	2.703%
20	19.839	2842	2848	2853	rBV	13178885	15766746	100.00%	17.904%
21	20.616	2976	2980	2985	rBV4	147365	240292	1.52%	0.273%
22	21.074	3054	3058	3065	rBV	820703	1060297	6.72%	1.204%
23	21.363	3102	3107	3118	rBV	3358681	4329610	27.46%	4.917%
24	21.516	3130	3133	3138	rVB	183491	209638	1.33%	0.238%
25	21.974	3208	3211	3220	rVB2	252477	416911	2.64%	0.473%
26	22.480	3294	3297	3303	rVB	296529	395197	2.51%	0.449%
27	22.621	3318	3321	3325	rVB	266354	358123	2.27%	0.407%
28	23.039	3389	3392	3398	rVB	342471	507335	3.22%	0.576%
29	23.774	3511	3517	3531	rVB2	2147429	4556304	28.90%	5.174%

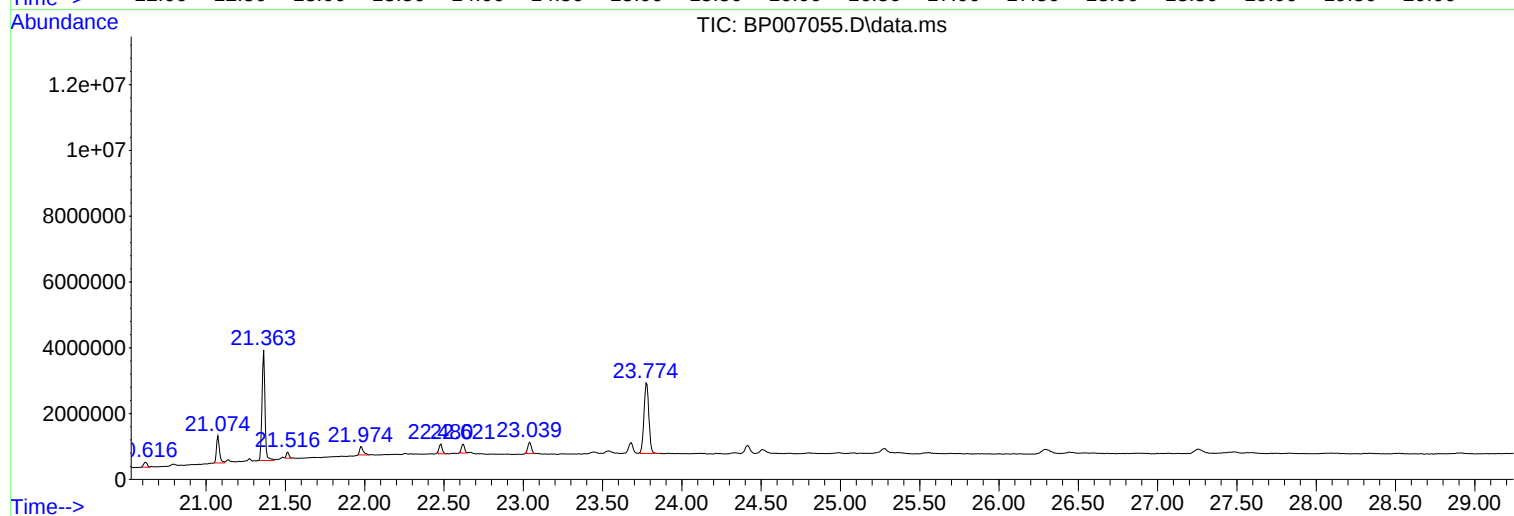
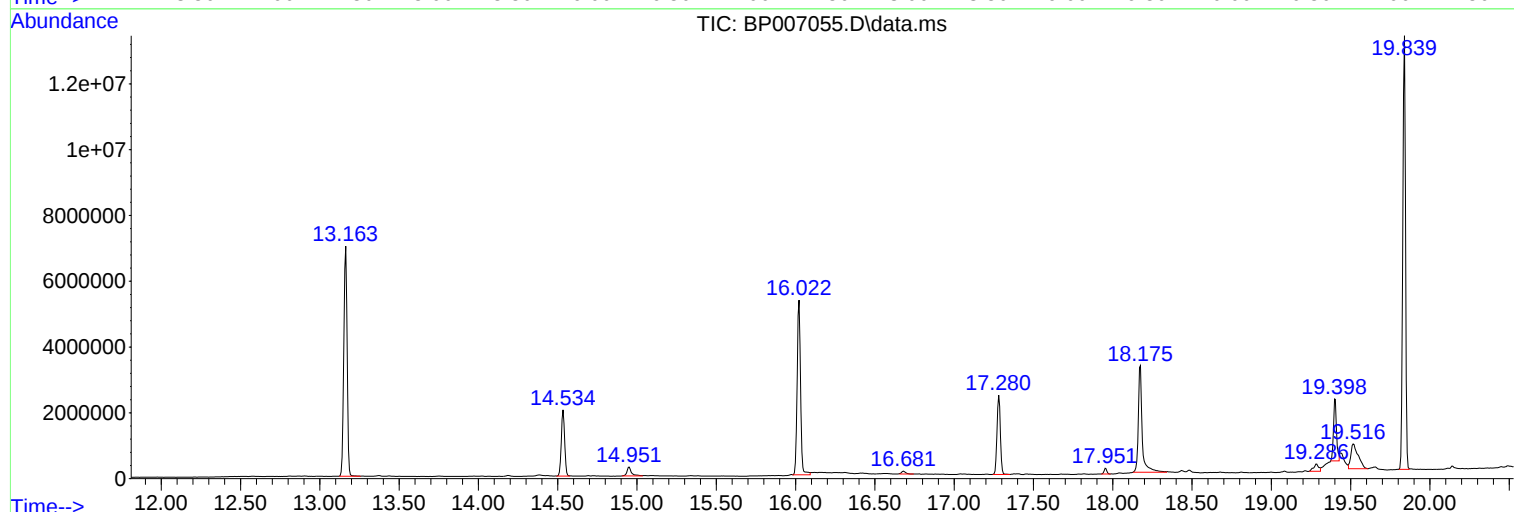
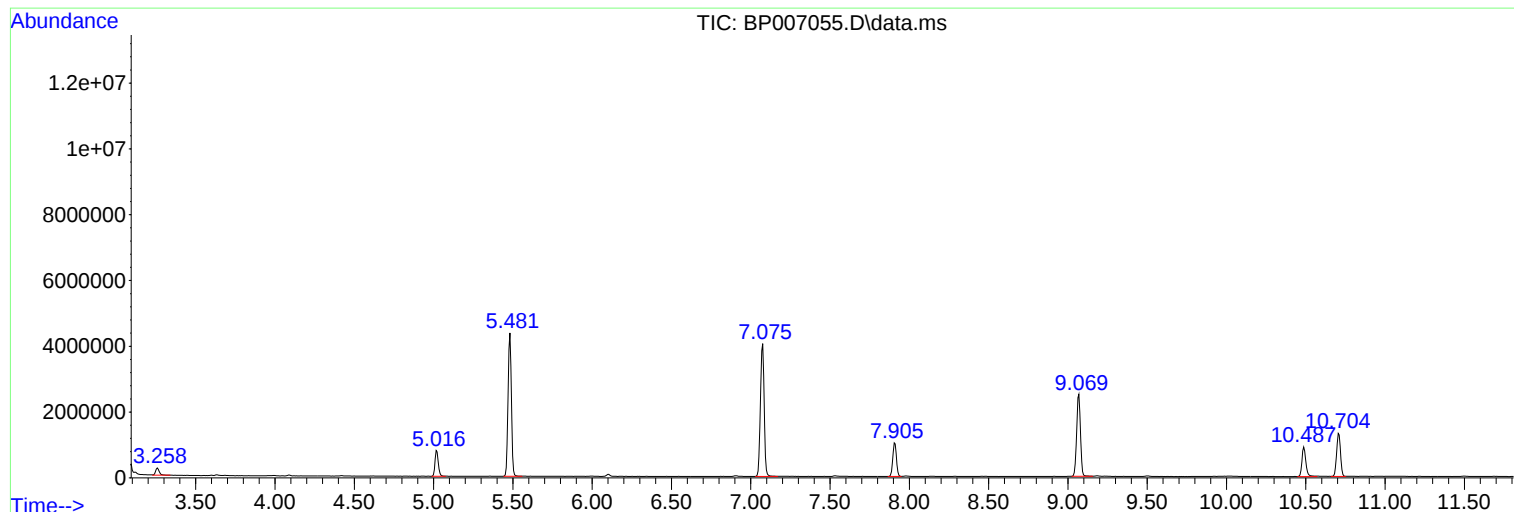
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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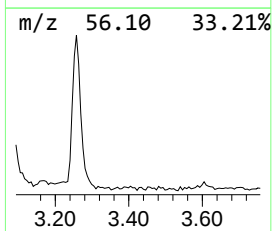
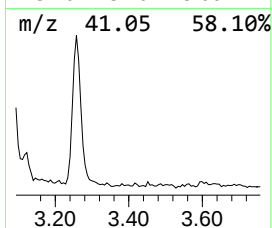
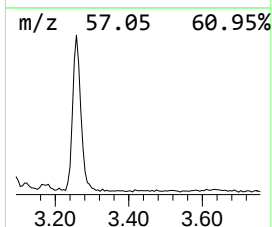
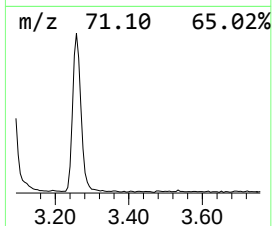
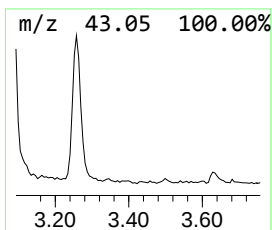
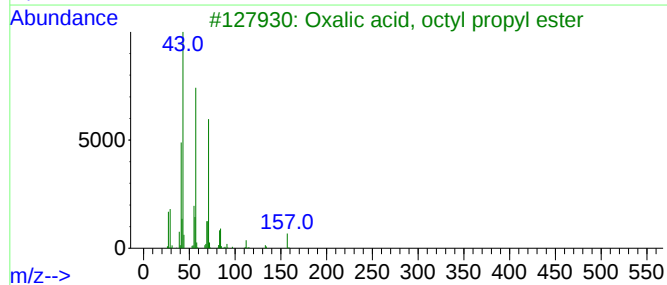
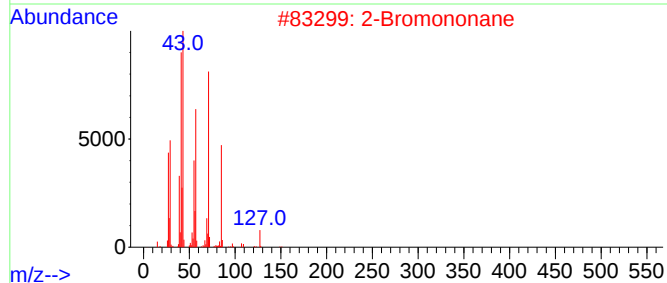
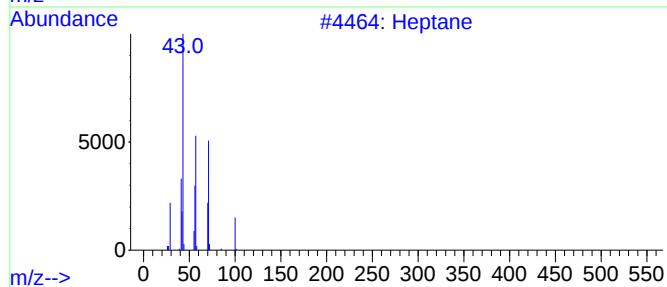
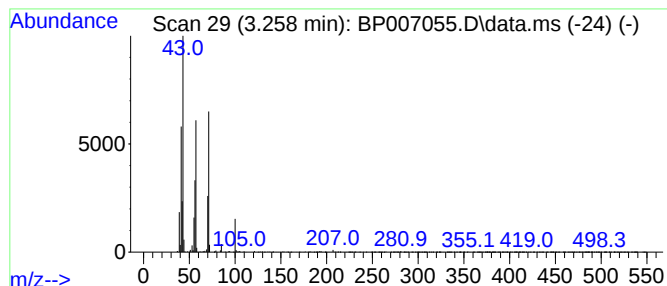
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	4.32 ng	352349	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			2-Bromononane	206	C9H19Br	002216-35-5	53
3			Oxalic acid, octyl propyl ester	244	C13H24O4	1010309-26-1	50
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	50
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	47



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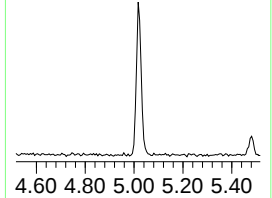
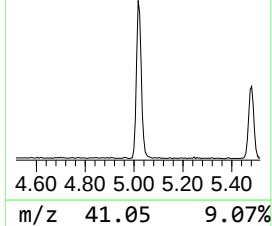
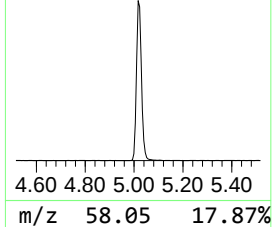
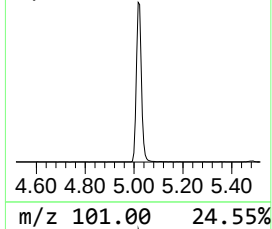
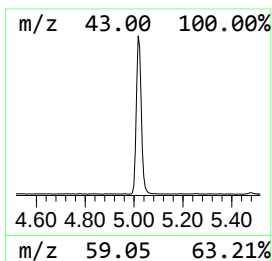
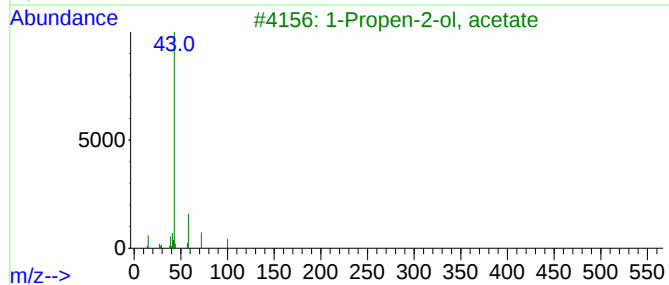
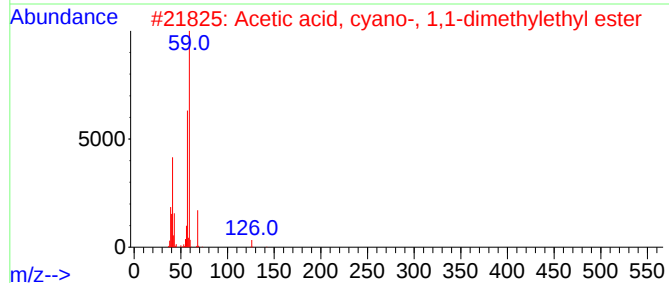
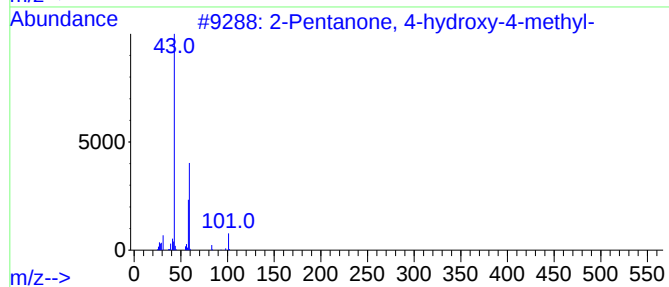
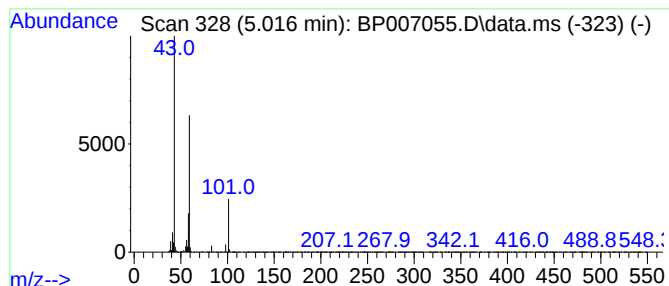
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	13.79 ng	1123490	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	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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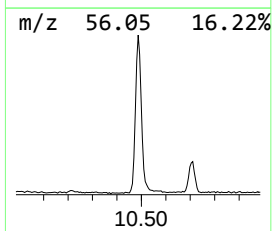
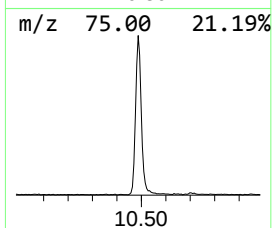
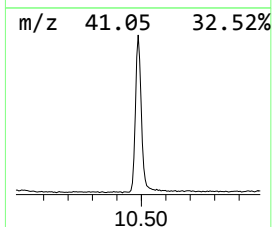
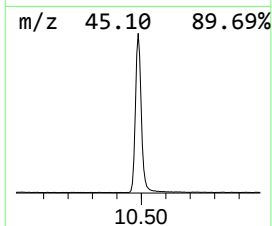
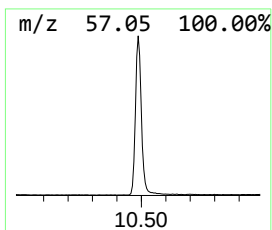
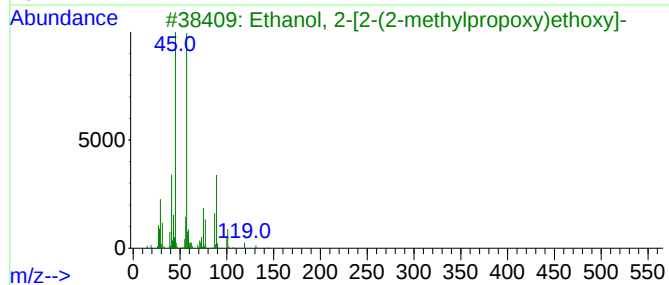
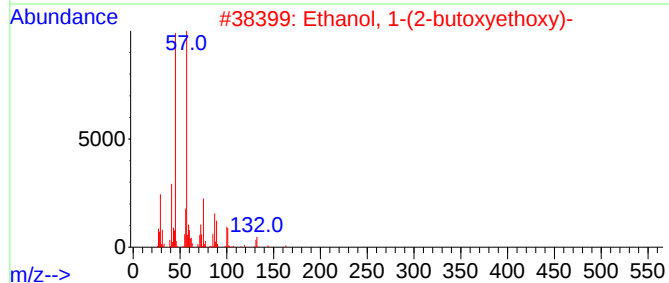
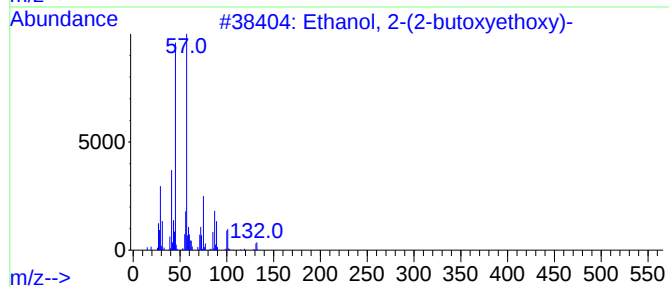
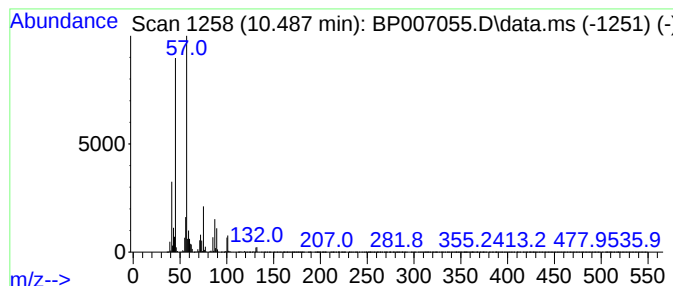
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	13.93 ng	1539120	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	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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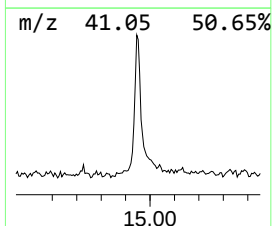
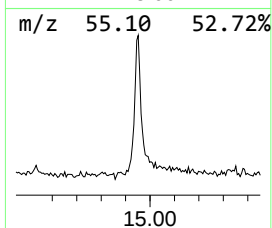
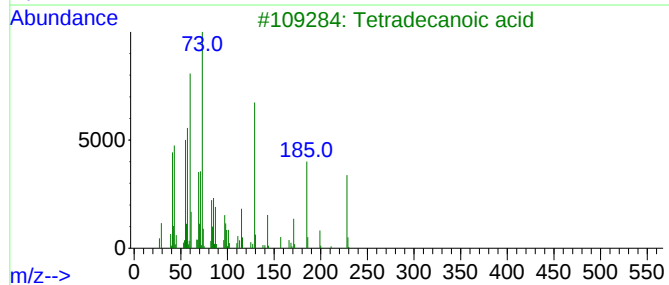
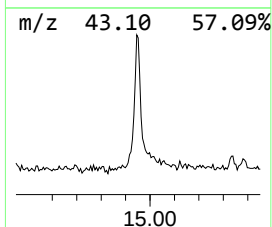
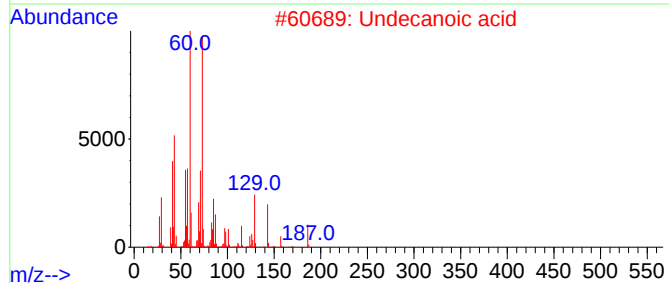
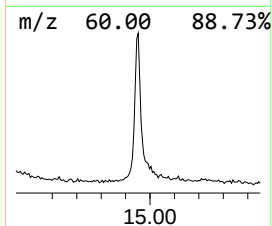
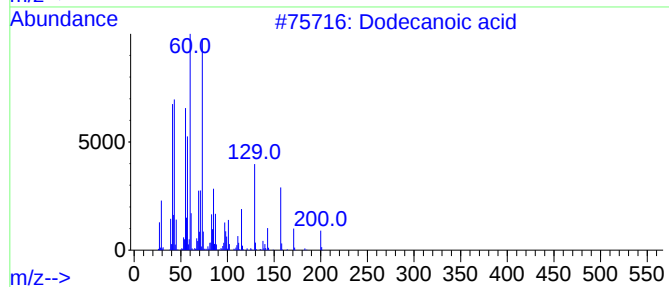
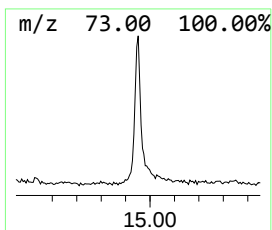
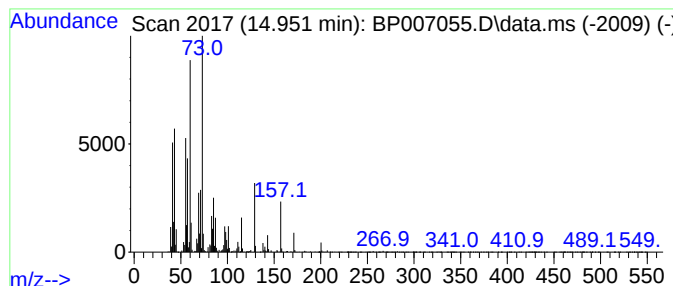
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Peak Number 4 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	3.68 ng	539668	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Octanoic acid	144	C8H16O2	000124-07-2	53
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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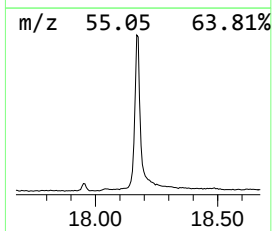
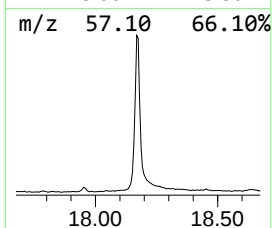
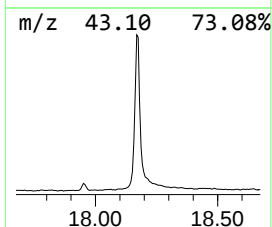
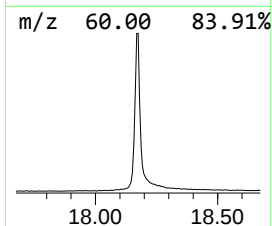
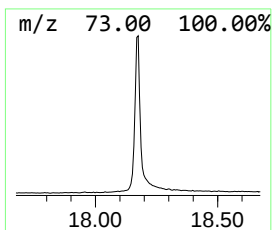
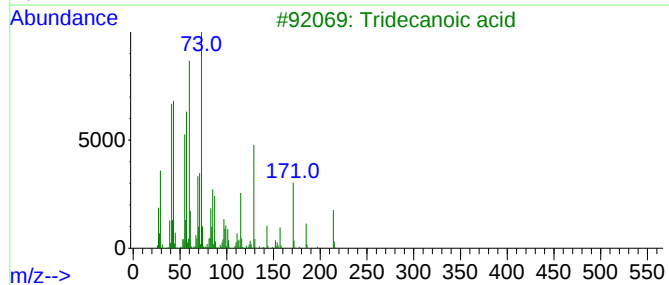
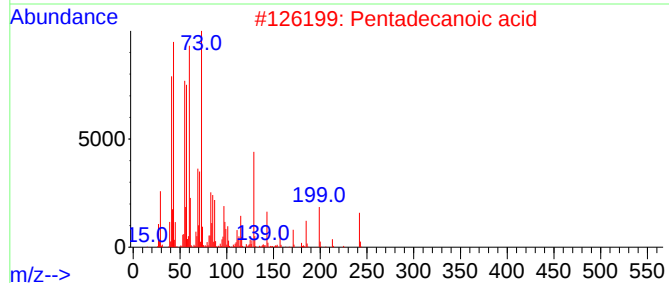
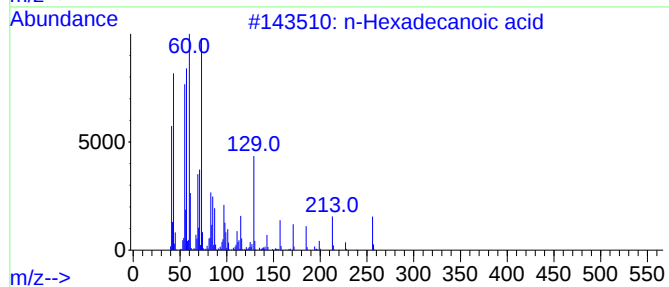
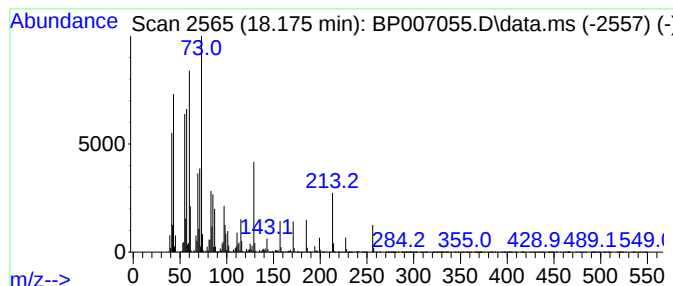
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	31.18 ng	5498540	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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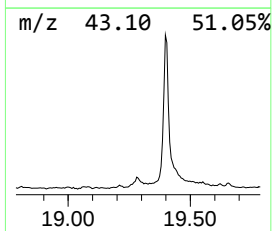
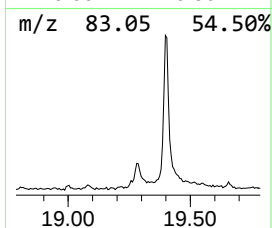
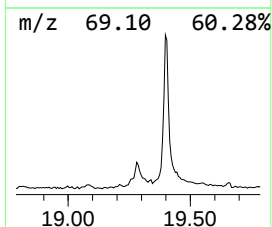
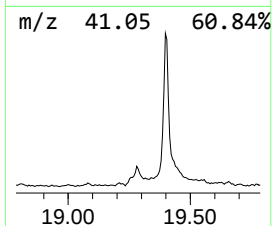
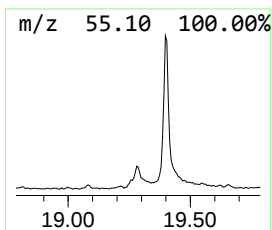
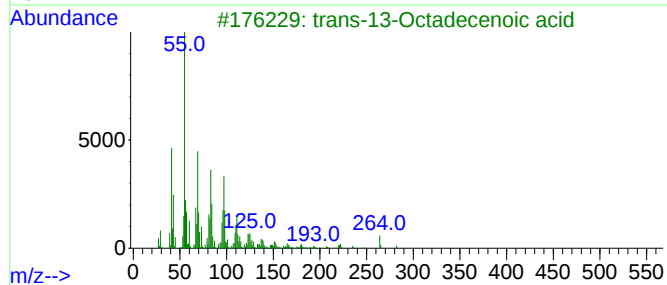
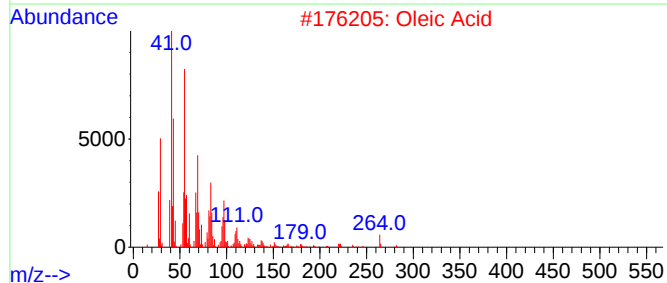
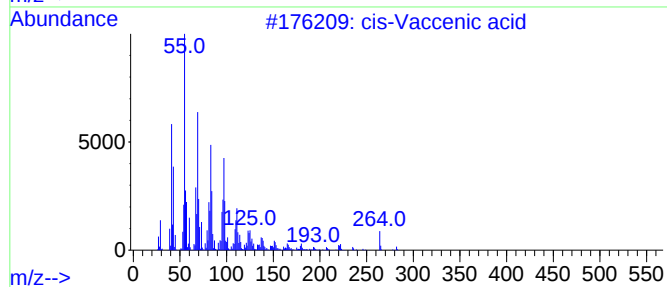
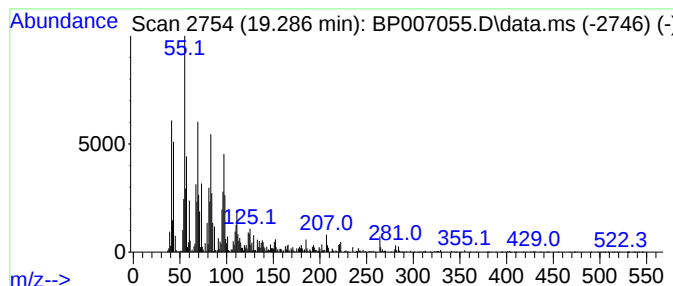
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-Vaccenic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	2.91 ng	513822	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2			Oleic Acid	282	C18H34O2	000112-80-1	99
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
5			9-Octadecenoic acid	282	C18H34O2	002027-47-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007055.D
Acq On : 20 Sep 2021 18:01
Operator : CG/JU
Sample : M3687-29
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A004145

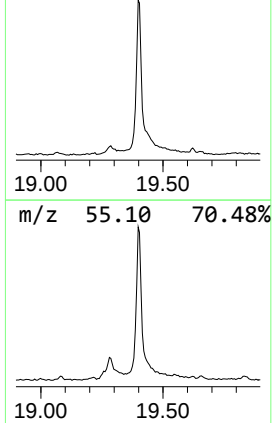
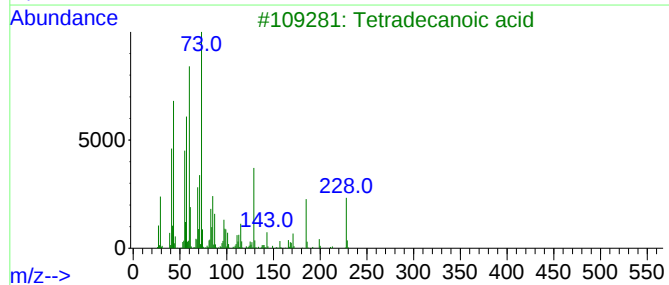
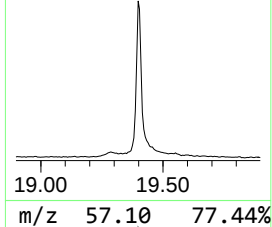
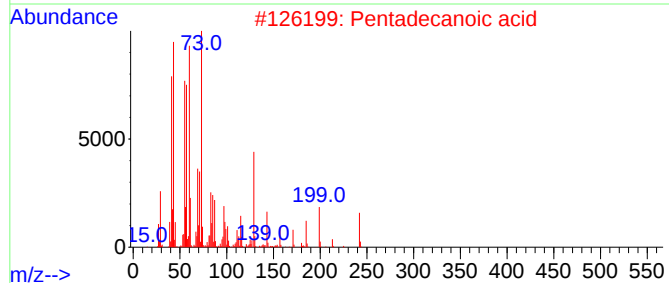
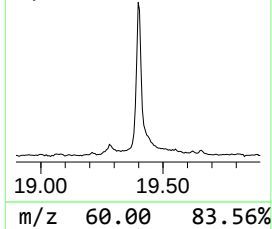
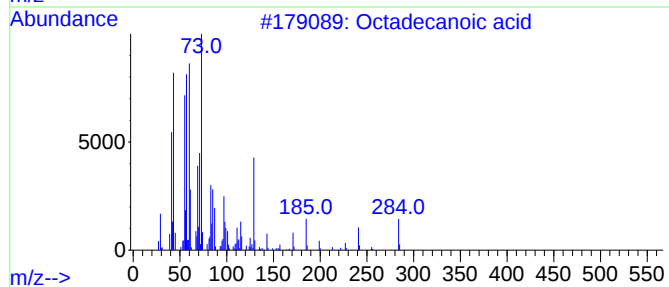
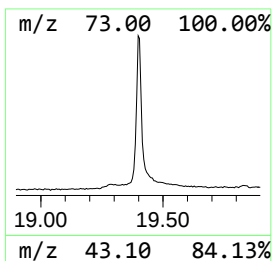
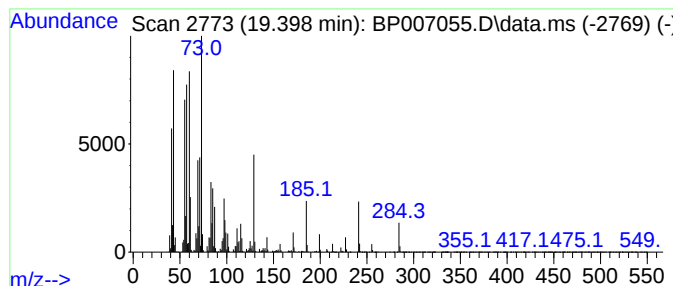
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	11.78 ng	2549880	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007055.D
Acq On : 20 Sep 2021 18:01
Operator : CG/JU
Sample : M3687-29
Misc :
ALS Vial : 4 Sample Multiplier: 1

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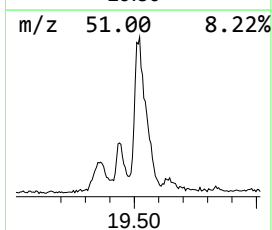
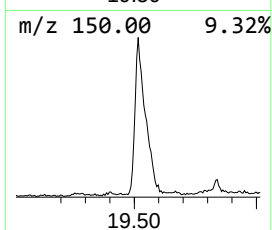
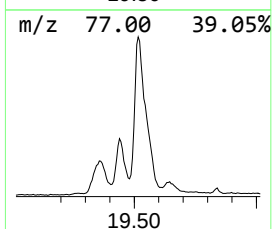
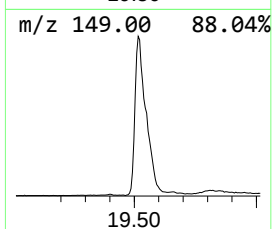
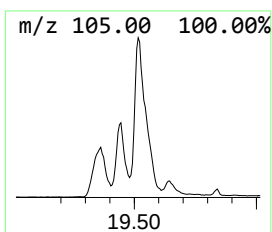
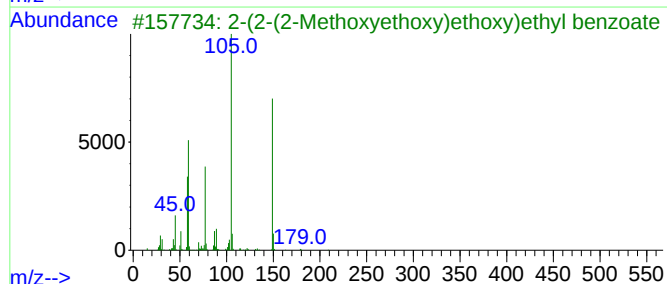
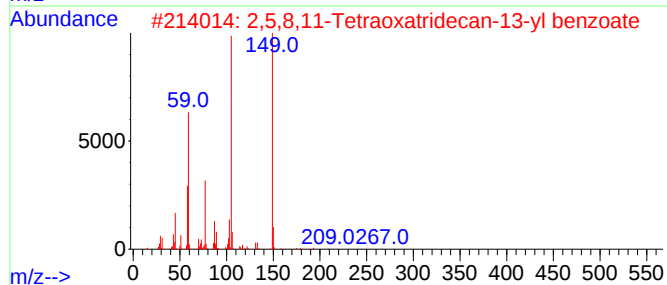
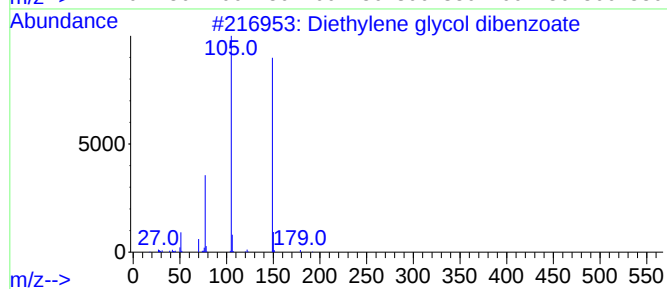
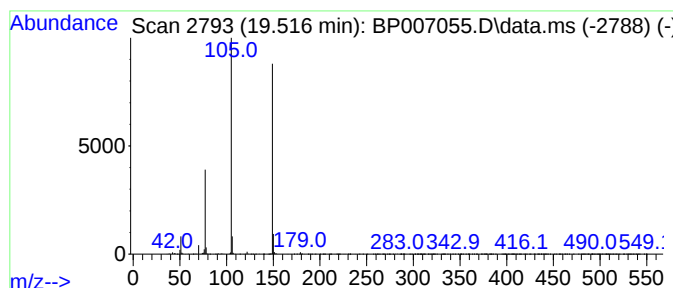
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	11.00 ng	2380390	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
3			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	72
5			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007055.D
Acq On : 20 Sep 2021 18:01
Operator : CG/JU
Sample : M3687-29
Misc :
ALS Vial : 4 Sample Multiplier: 1

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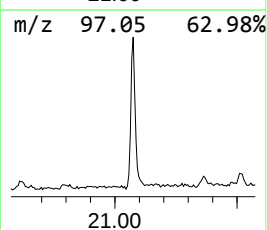
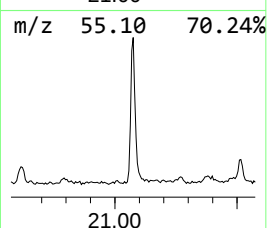
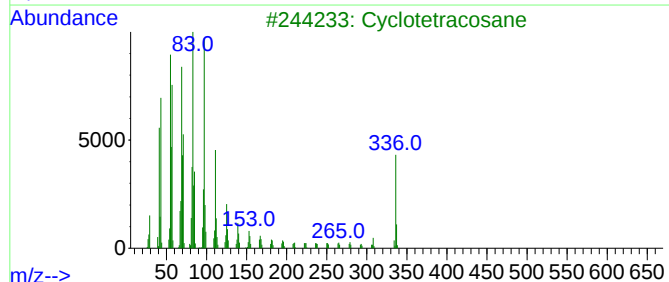
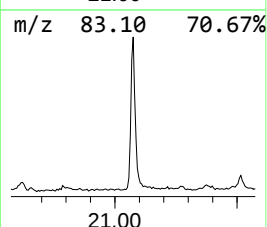
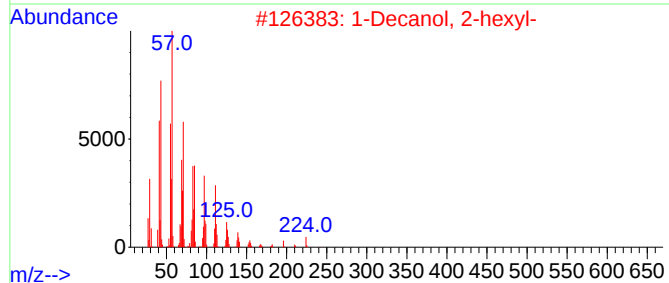
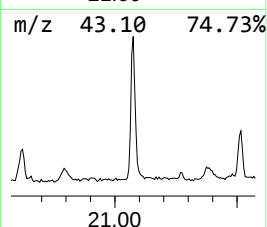
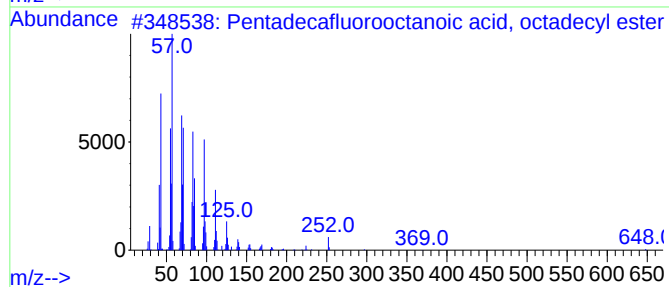
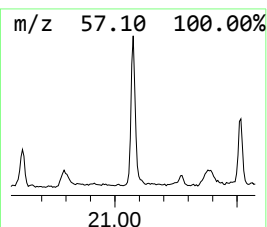
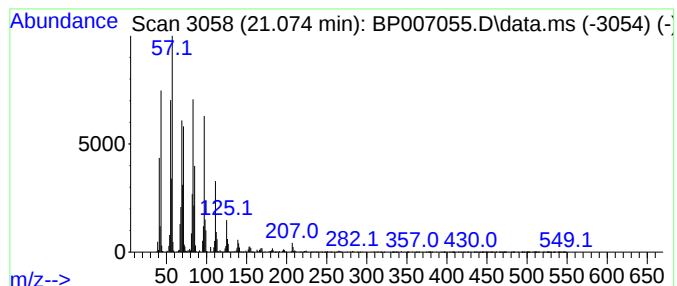
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	4.90 ng	1060300	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	93
3			Cyclotetracosane	336	C24H48	000297-03-0	93
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007055.D
Acq On : 20 Sep 2021 18:01
Operator : CG/JU
Sample : M3687-29
Misc :
ALS Vial : 4 Sample Multiplier: 1

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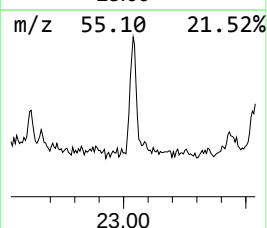
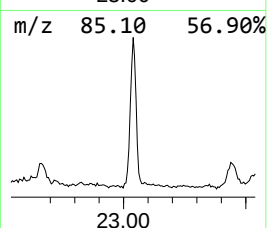
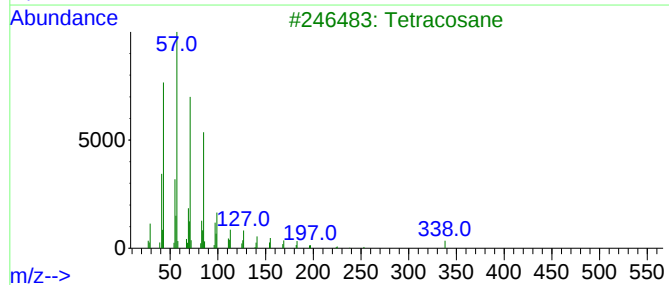
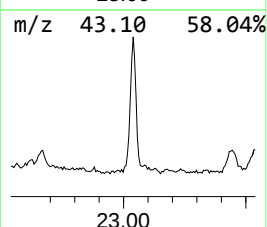
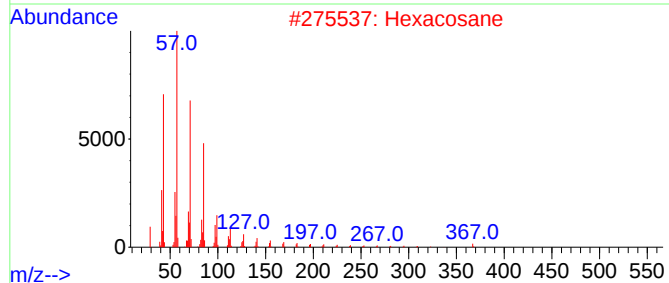
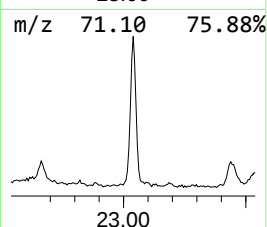
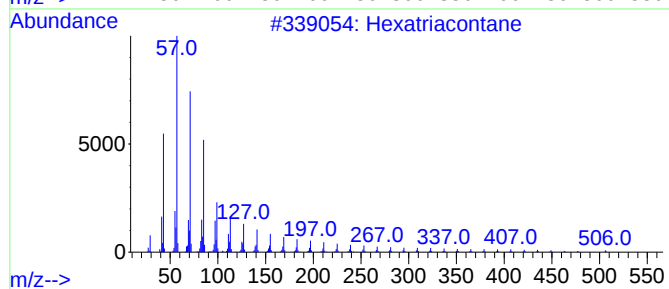
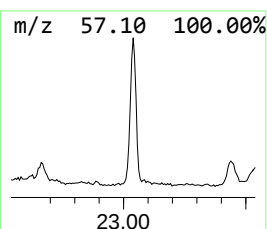
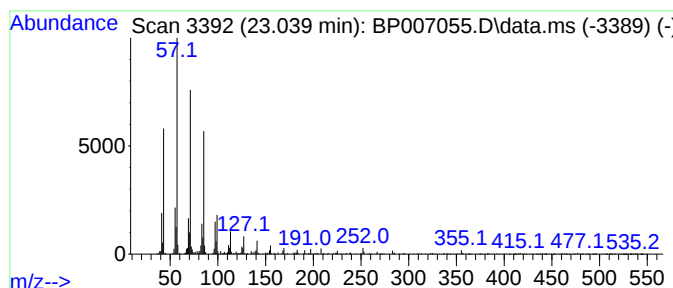
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexatriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.039	2.23 ng	507335	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
5			Docosane, 11-decyl-	451	C32H66	055401-55-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007055.D
Acq On : 20 Sep 2021 18:01
Operator : CG/JU
Sample : M3687-29
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.016	13.8	ng	1123490	1	7.905	1629660	20.0
Ethanol, 2-(2-b...	10.487	13.9	ng	1539120	2	10.704	2210460	20.0
Dodecanoic acid	14.951	3.7	ng	539668	3	14.534	2933600	20.0
n-Hexadecanoic ...	18.175	31.2	ng	5498540	4	17.281	3527160	20.0
cis-Vaccenic acid	19.286	2.9	ng	513822	4	17.281	3527160	20.0
Octadecanoic acid	19.398	11.8	ng	2549880	5	21.363	4329610	20.0
Diethylene glyc...	19.516	11.0	ng	2380390	5	21.363	4329610	20.0
Pentadecafluoro...	21.074	4.9	ng	1060300	5	21.363	4329610	20.0
Hexatriacontane	23.039	2.2	ng	507335	6	23.774	4556300	20.0