

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071321\
 Data File : BP006208.D
 Acq On : 13 Jul 2021 19:26
 Operator : CG/JU
 Sample : M3015-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RED-FRAC-TANK

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-BP070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.964	315	319	326	rBV	57602	90127	1.20%	0.266%
2	5.440	395	400	421	rBV	232520	471208	6.28%	1.389%
3	7.058	668	675	692	rBV	145902	330216	4.40%	0.974%
4	7.852	799	810	819	rBV	593106	984049	13.12%	2.902%
5	8.116	849	855	871	rBV	283327	717008	9.56%	2.114%
6	8.952	988	997	1002	rBV2	45011	79612	1.06%	0.235%
7	9.022	1002	1009	1028	rBV	1286293	2316610	30.88%	6.831%
8	10.440	1243	1250	1275	rBV	771361	1852000	24.69%	5.461%
9	10.651	1279	1286	1291	rBV	808836	1382853	18.43%	4.078%
10	10.704	1291	1295	1304	rVB	706246	1188414	15.84%	3.504%
11	12.351	1566	1575	1591	rBV2	55013	182520	2.43%	0.538%
12	13.110	1697	1704	1718	rBV	3131274	5019551	66.91%	14.801%
13	14.487	1931	1938	1946	rBV	1136176	1662388	22.16%	4.902%
14	15.986	2187	2193	2208	rVB	956413	1550344	20.67%	4.571%
15	17.239	2400	2406	2412	rBV	1301594	1829676	24.39%	5.395%
16	17.898	2514	2518	2523	rVB	141186	172135	2.29%	0.508%
17	18.122	2552	2556	2564	rBV	337126	507451	6.76%	1.496%
18	19.028	2707	2710	2714	rVB	84305	93798	1.25%	0.277%
19	19.351	2761	2765	2775	rBV	142659	219996	2.93%	0.649%
20	19.622	2806	2811	2817	rBV	285411	412589	5.50%	1.217%
21	19.680	2818	2821	2827	rVB	88520	106768	1.42%	0.315%
22	19.792	2834	2840	2847	rBV	6145424	7501551	100.00%	22.120%
23	20.216	2909	2912	2916	rBV	101731	104493	1.39%	0.308%
24	20.716	2994	2997	3001	rBV	81685	83059	1.11%	0.245%
25	21.022	3045	3049	3057	rBV2	442740	668231	8.91%	1.970%
26	21.316	3095	3099	3108	rBV	1501760	1876604	25.02%	5.533%
27	22.521	3301	3304	3311	rVB	227142	332201	4.43%	0.980%
28	23.698	3498	3504	3514	rVB2	1060547	2178160	29.04%	6.423%

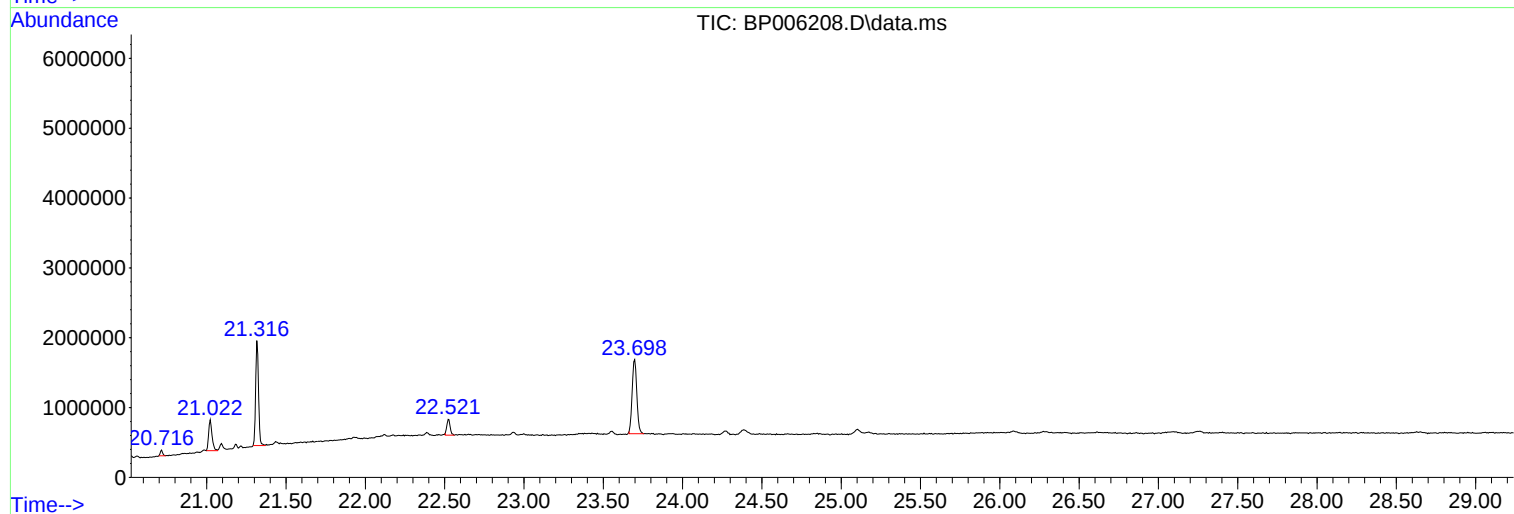
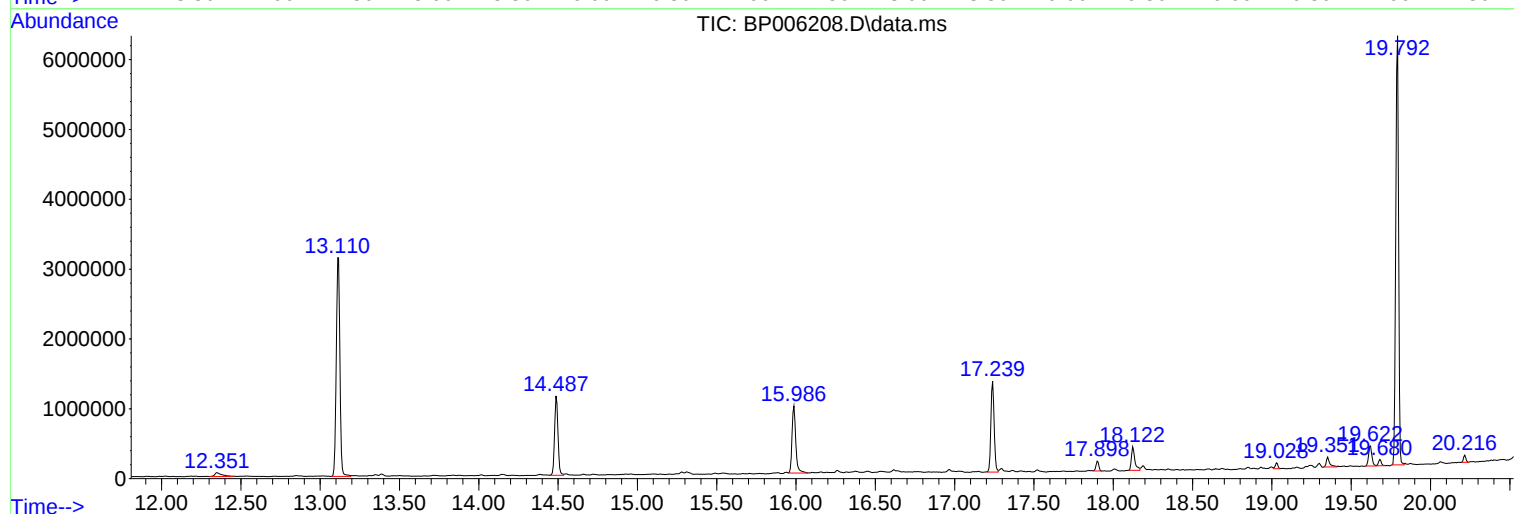
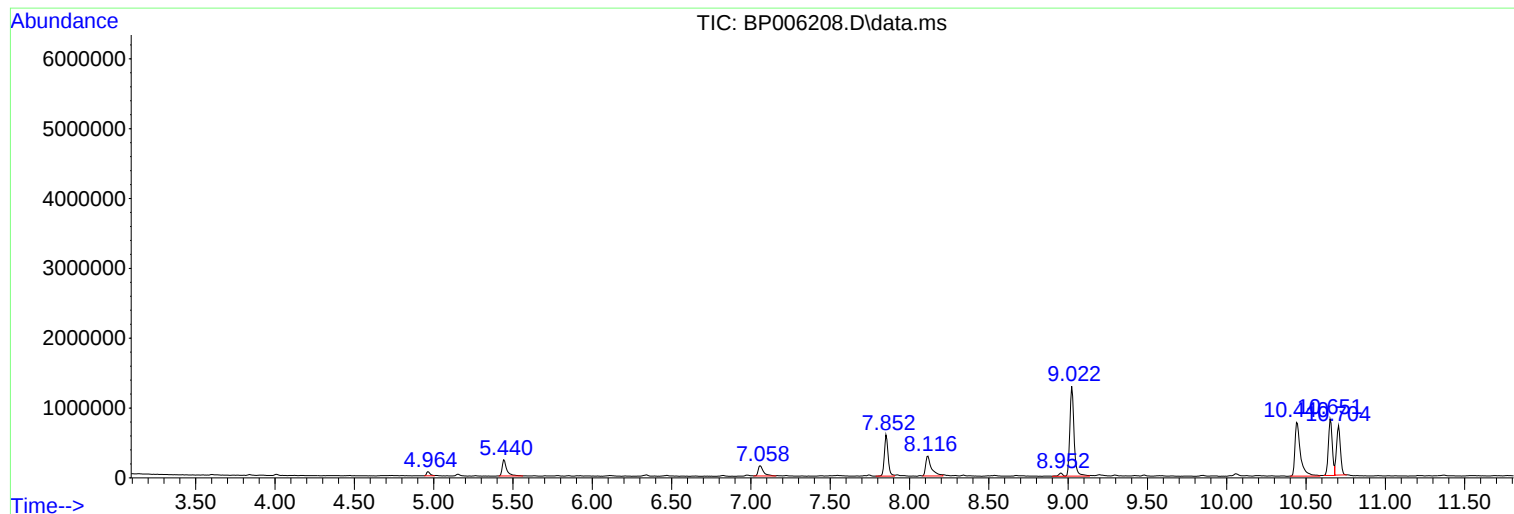
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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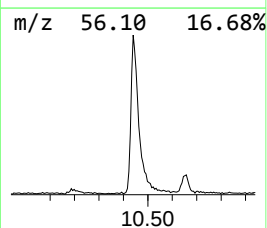
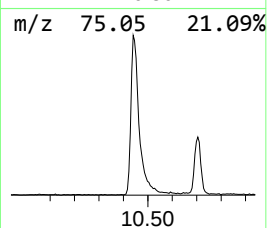
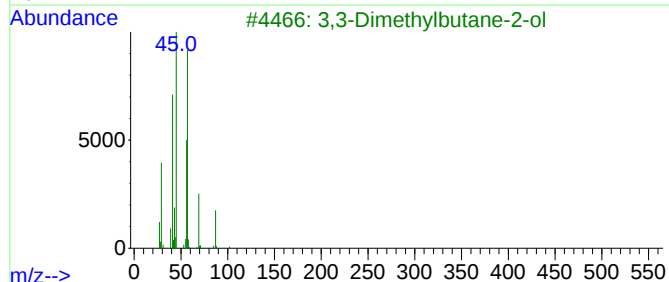
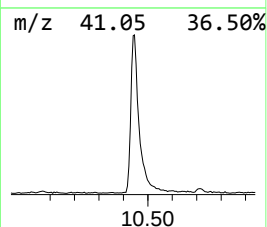
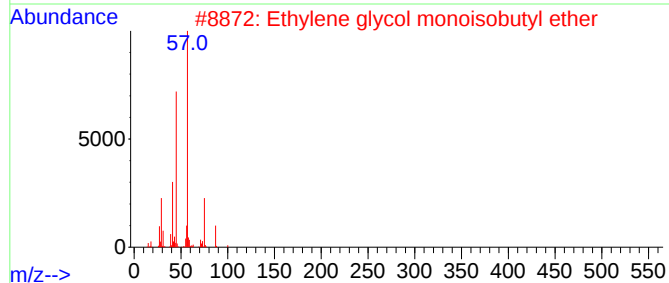
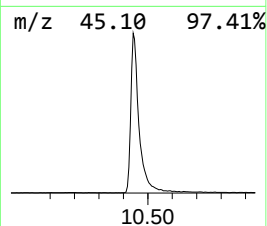
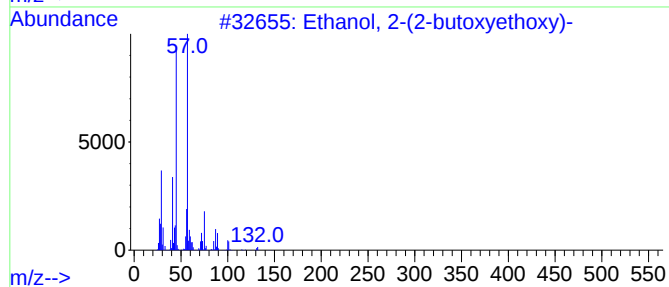
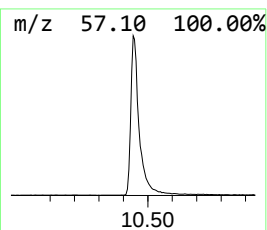
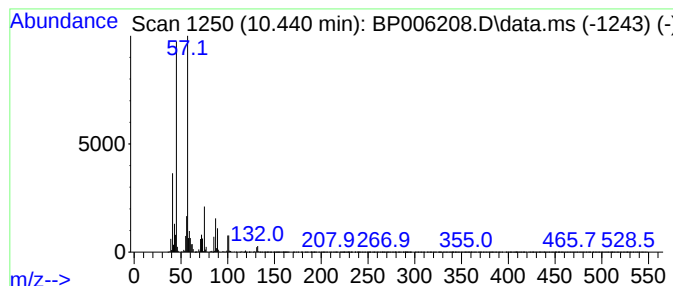
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.440	26.79 ng	1852000	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Di-sec-butyl ether	130	C8H18O	006863-58-7	50



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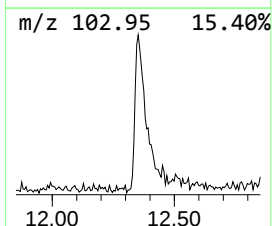
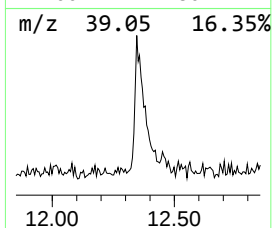
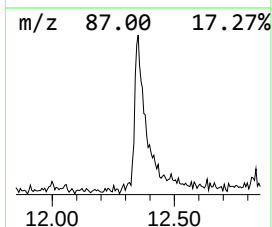
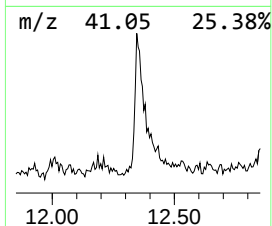
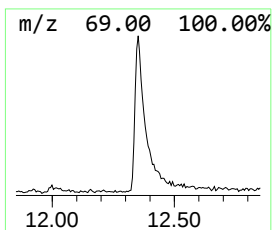
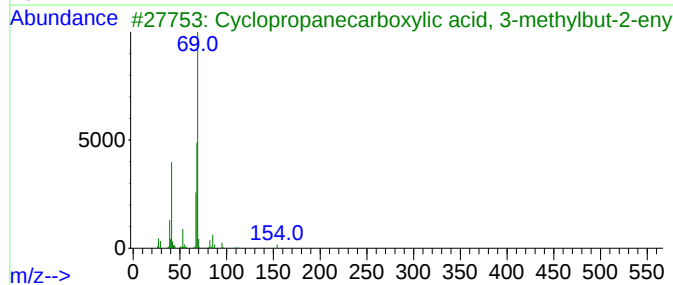
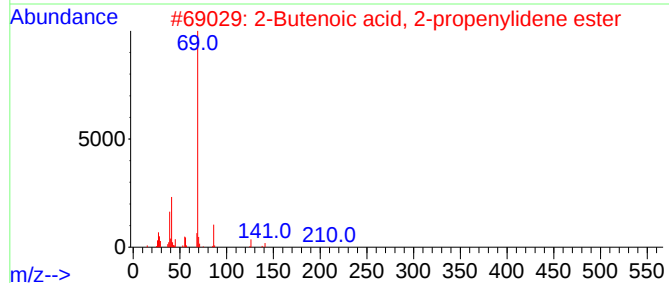
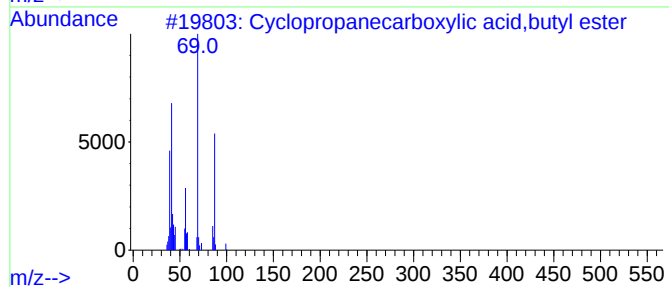
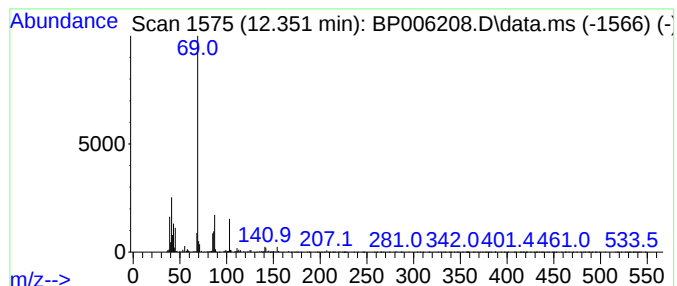
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.351	2.64 ng	182520	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	59
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	52
3			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	50
4			Cyclopropanecarboxylic acid, pen...	150	C9H10O2	1000299-37-5	38
5			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38



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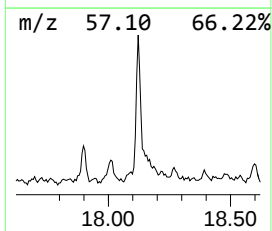
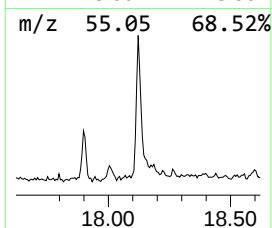
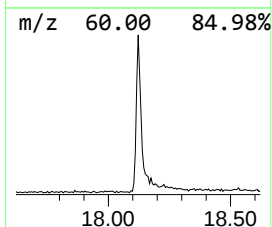
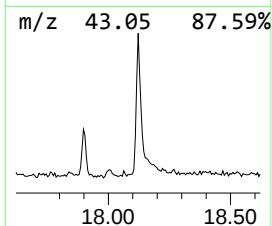
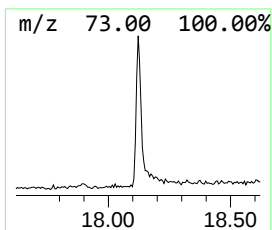
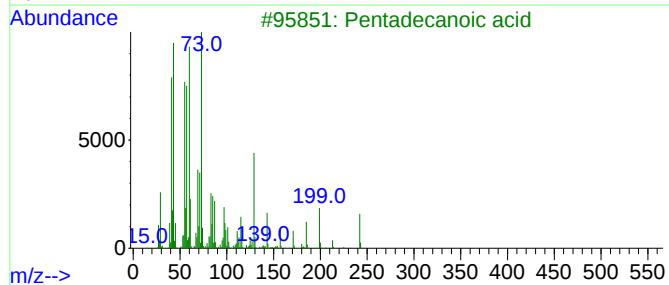
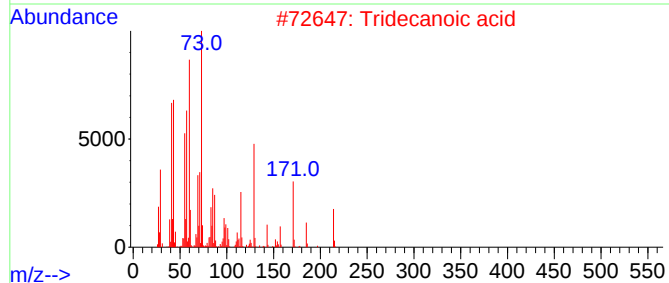
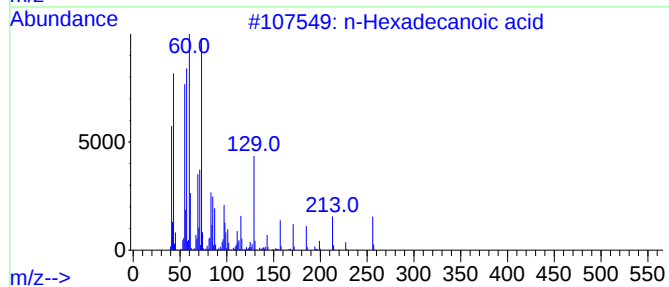
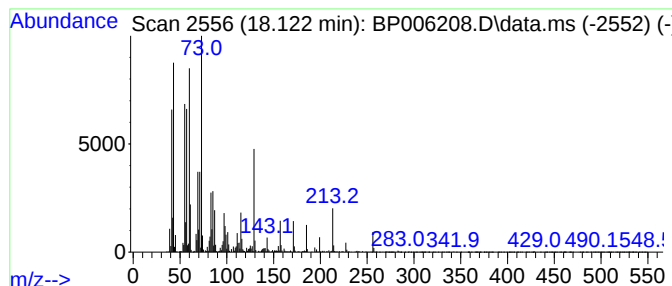
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	5.55 ng	507451	Phenanthrene-d10	17.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	70



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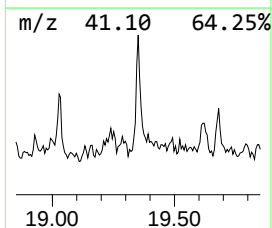
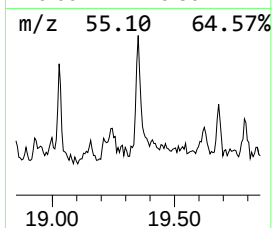
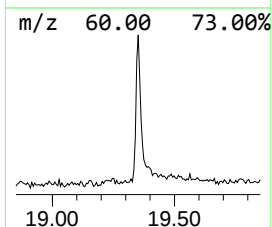
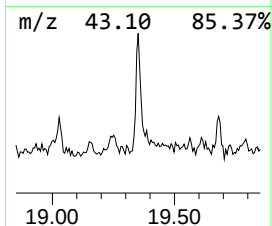
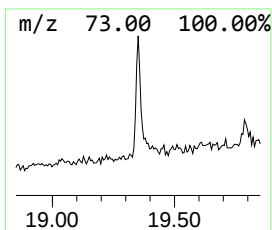
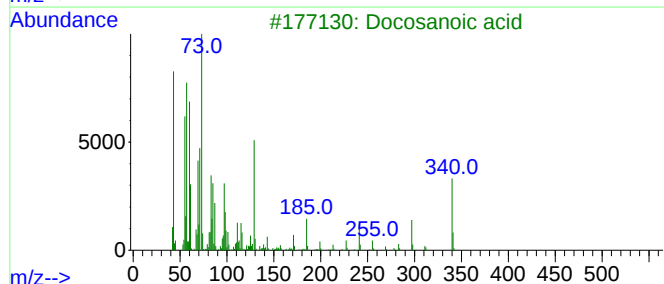
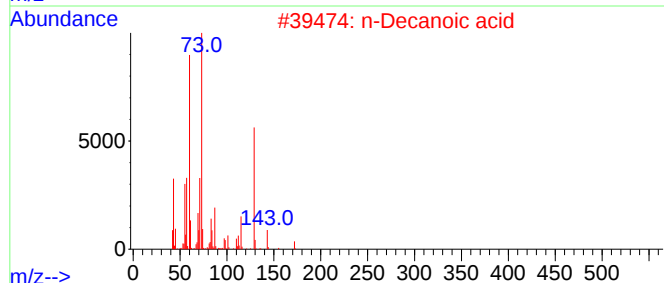
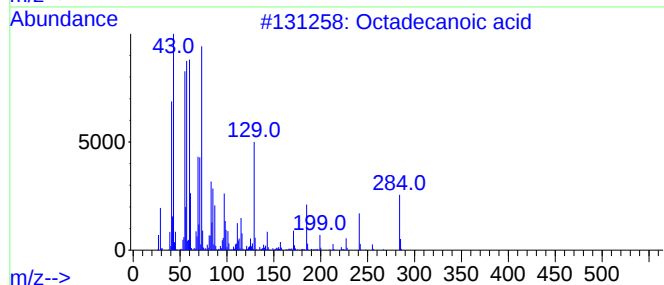
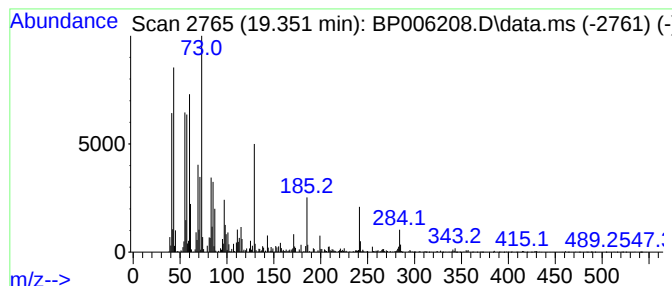
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	2.34 ng	219996	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	95
3			Docosanoic acid	340	C22H44O2	000112-85-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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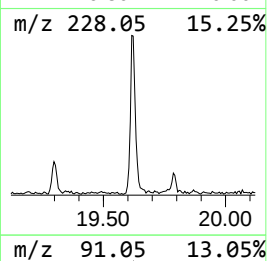
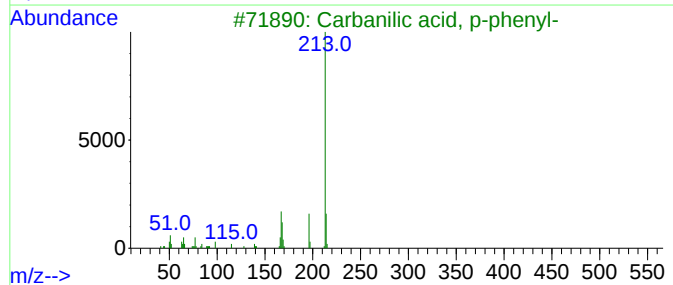
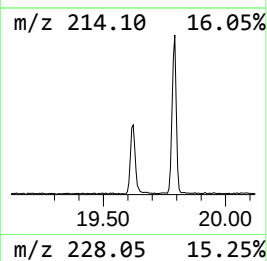
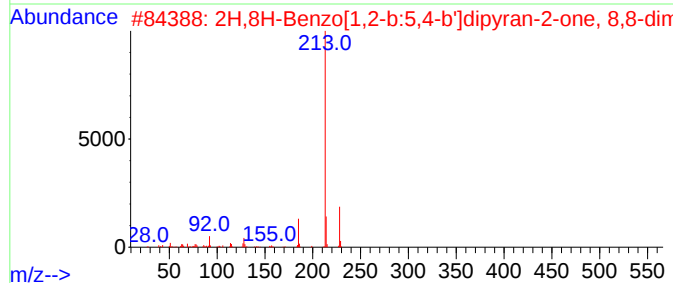
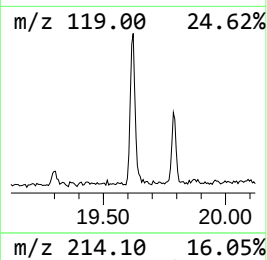
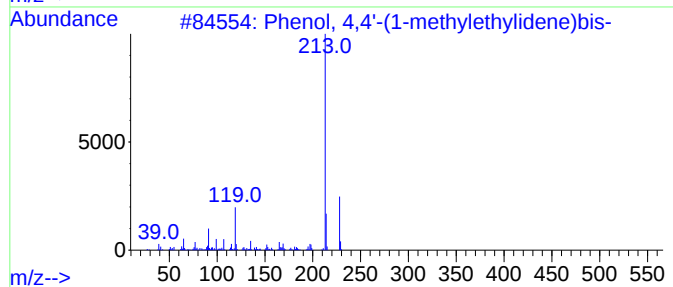
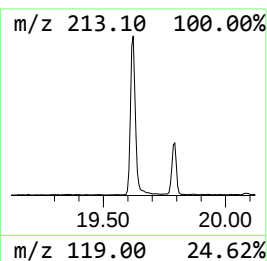
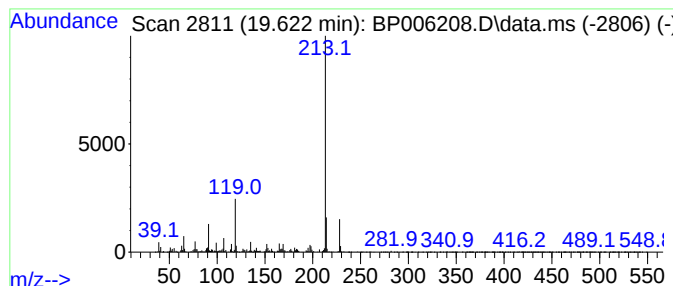
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.622	4.40 ng	412589	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
3			Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
4			Acridine, 9-chloro-	213	C13H8ClN	001207-69-8	50
5			Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	50



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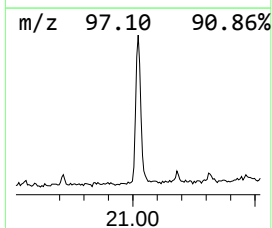
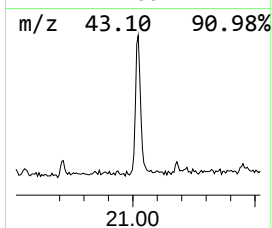
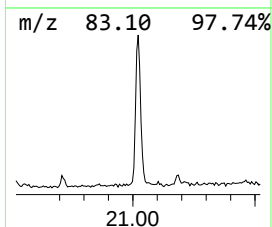
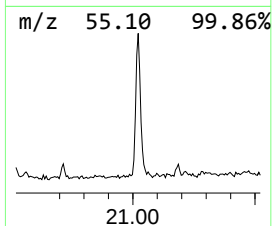
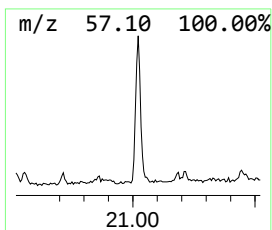
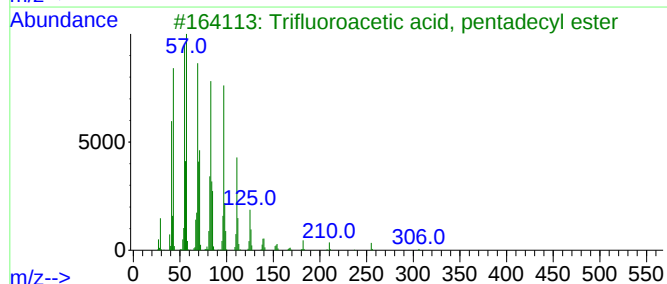
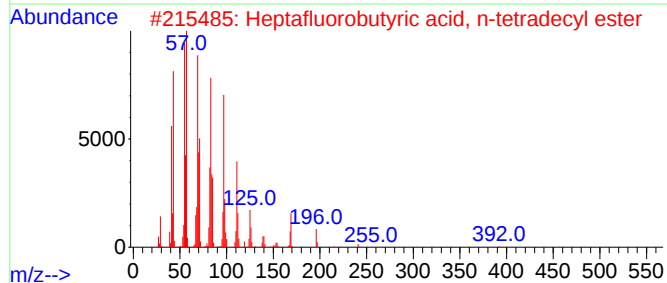
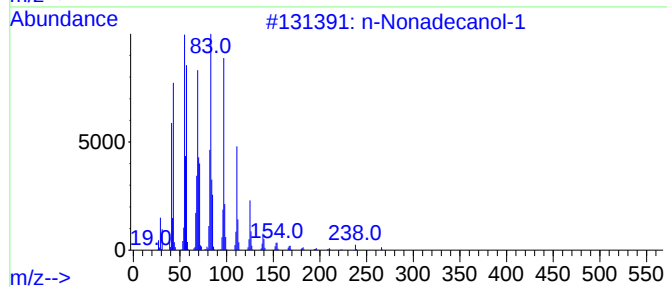
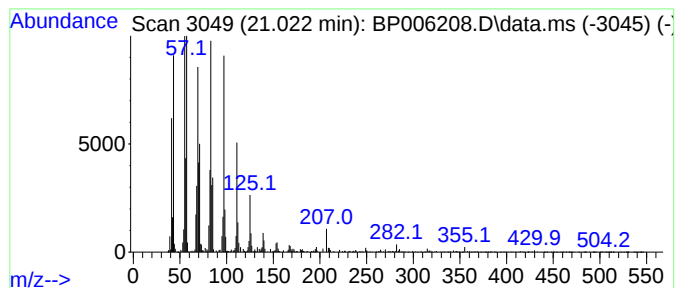
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	7.12 ng	668231	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071321\
Data File : BP006208.D
Acq On : 13 Jul 2021 19:26
Operator : CG/JU
Sample : M3015-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RED-FRAC-TANK

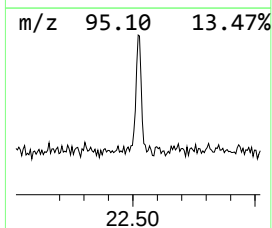
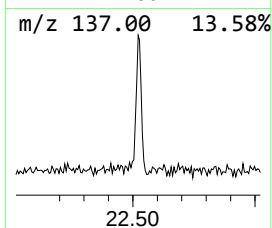
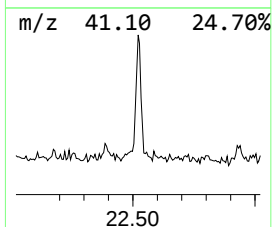
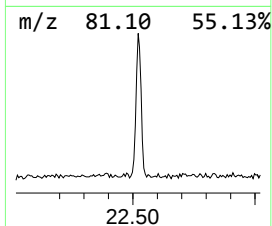
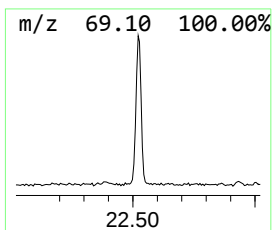
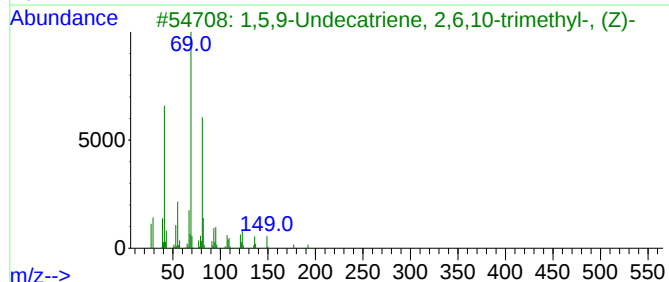
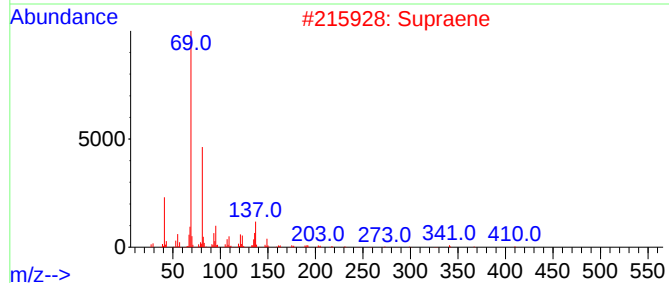
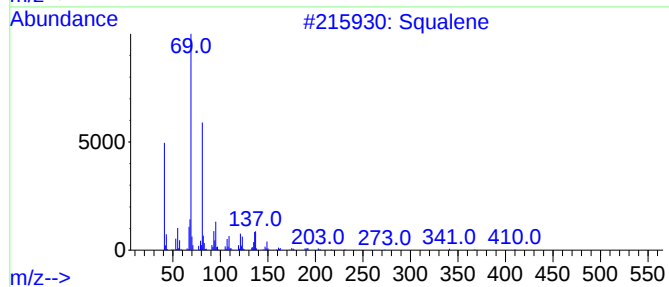
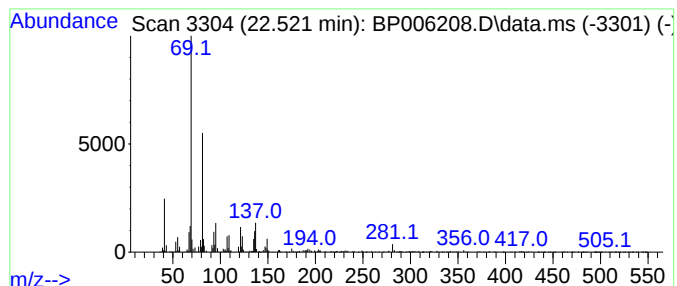
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.521	3.05 ng	332201	Perylene-d12	23.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	94
2			Supraene	410	C30H50	007683-64-9	93
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071321\
Data File : BP006208.D
Acq On : 13 Jul 2021 19:26
Operator : CG/JU
Sample : M3015-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RED-FRAC-TANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.440	26.8	ng	1852000	2	10.652	1382850	20.0
Cyclopropanecar...	12.351	2.6	ng	182520	2	10.652	1382850	20.0
n-Hexadecanoic ...	18.122	5.5	ng	507451	4	17.239	1829680	20.0
Octadecanoic acid	19.351	2.3	ng	219996	5	21.316	1876600	20.0
Phenol, 4,4'-(1...	19.622	4.4	ng	412589	5	21.316	1876600	20.0
n-Nonadecanol-1	21.022	7.1	ng	668231	5	21.316	1876600	20.0
Squalene	22.521	3.0	ng	332201	6	23.698	2178160	20.0