

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
 Data File : BP006148.D
 Acq On : 08 Jul 2021 19:51
 Operator : CG/JU
 Sample : M2944-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BU-03-070621

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: BP006148.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	318	323	334	rBV	62747	104910	1.10%	0.157%
2	5.452	396	402	428	rBV	2627445	4205788	44.13%	6.309%
3	7.058	669	675	701	rBV	2350628	4236873	44.46%	6.355%
4	7.875	806	814	826	rBV	692433	1146307	12.03%	1.719%
5	9.046	1005	1013	1030	rBV	1463529	2647592	27.78%	3.971%
6	10.675	1282	1290	1308	rBV	832275	1555235	16.32%	2.333%
7	13.134	1700	1708	1724	rBV	4205140	6133357	64.36%	9.200%
8	13.975	1845	1851	1863	rBV	262314	419349	4.40%	0.629%
9	14.510	1935	1942	1957	rVB	1270180	1890400	19.84%	2.836%
10	16.004	2189	2196	2216	rBV	2871432	4261173	44.71%	6.392%
11	17.257	2404	2409	2414	rBV	1324457	2002906	21.02%	3.004%
12	17.304	2414	2417	2422	rVB	87281	129096	1.35%	0.194%
13	17.922	2517	2522	2528	rVB	1180878	1360590	14.28%	2.041%
14	18.151	2555	2561	2570	rBV	852042	1300479	13.65%	1.951%
15	18.528	2618	2625	2628	rBV3	78079	172352	1.81%	0.259%
16	18.657	2644	2647	2653	rBV3	101821	138278	1.45%	0.207%
17	19.022	2704	2709	2712	rBV	7878928	9530100	100.00%	14.295%
18	19.057	2712	2715	2726	rVB2	6286664	7887865	82.77%	11.832%
19	19.181	2732	2736	2741	rVB	1073216	1201173	12.60%	1.802%
20	19.239	2742	2746	2747	rBV	376017	415511	4.36%	0.623%
21	19.263	2747	2750	2756	rVB2	641862	923507	9.69%	1.385%
22	19.375	2766	2769	2774	rBV2	167515	208304	2.19%	0.312%
23	19.622	2807	2811	2818	rVB	271463	457655	4.80%	0.686%
24	19.810	2838	2843	2849	rBV	6147368	7628052	80.04%	11.442%
25	20.245	2913	2917	2928	rBV3	176550	451095	4.73%	0.677%
26	21.045	3049	3053	3061	rVB2	824449	1230960	12.92%	1.846%
27	21.116	3061	3065	3070	rBV	343767	491616	5.16%	0.737%
28	21.339	3098	3103	3107	rBV	1726159	2243353	23.54%	3.365%
29	23.733	3504	3510	3517	rVB2	1219454	2292925	24.06%	3.439%

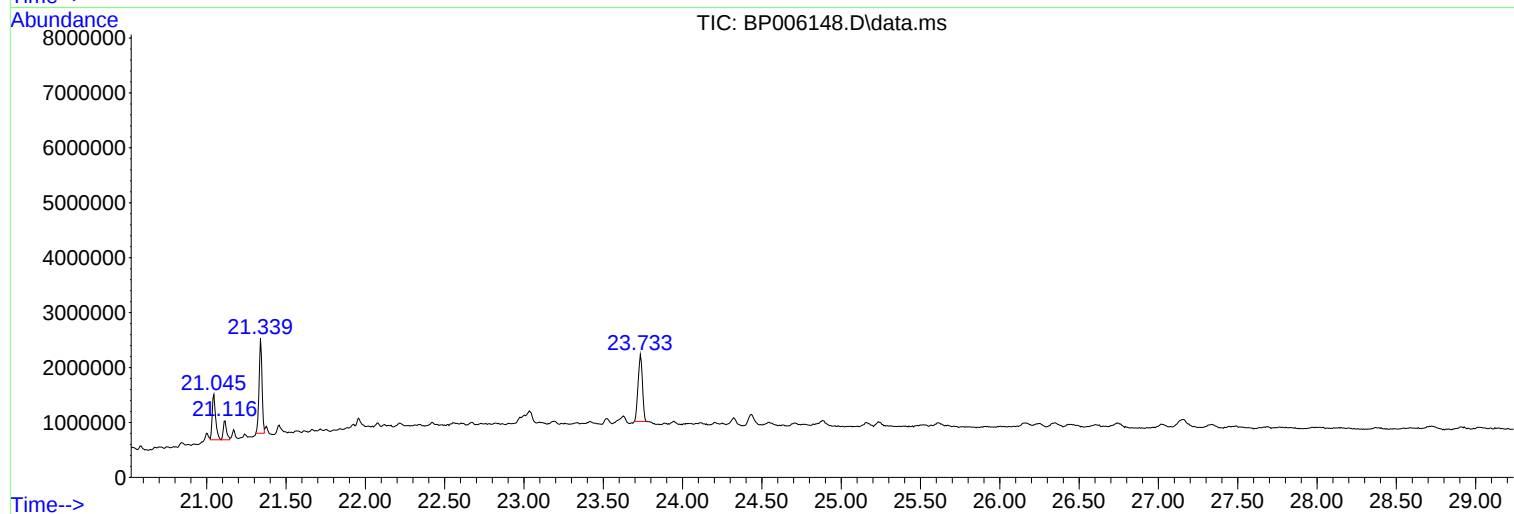
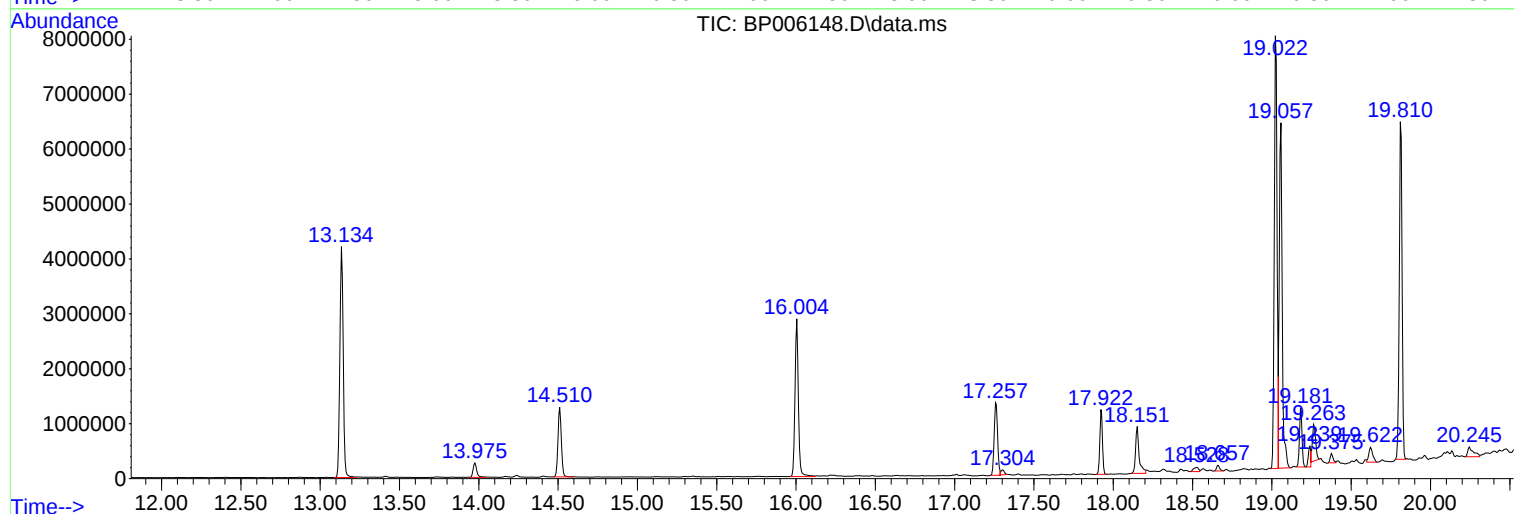
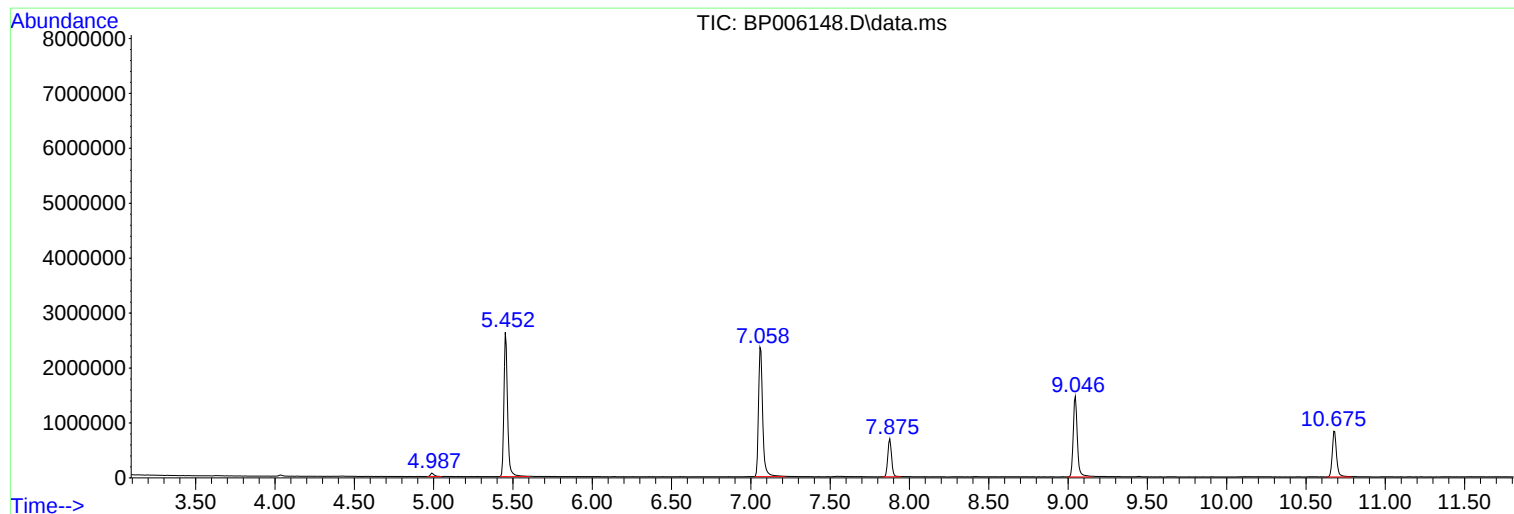
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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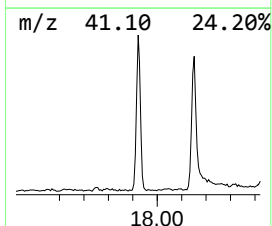
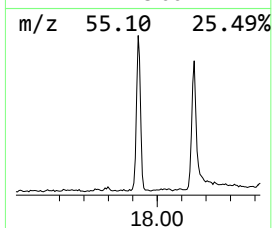
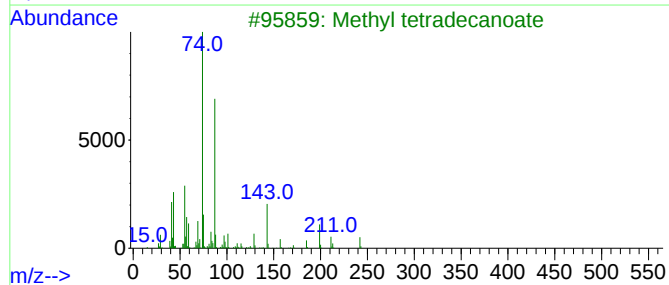
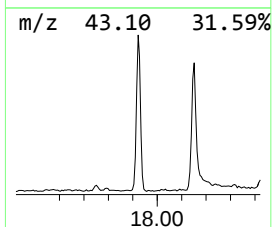
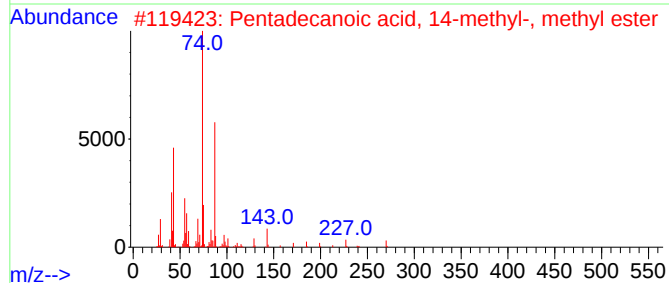
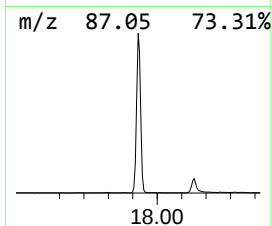
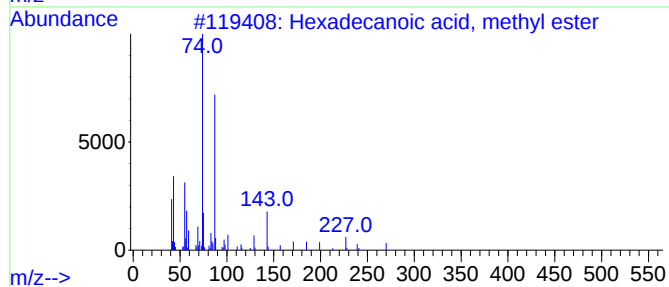
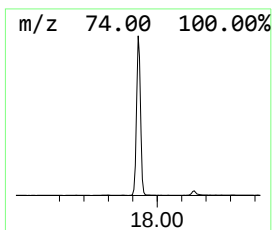
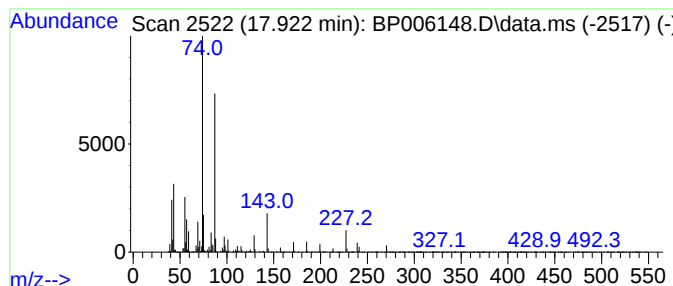
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.922	13.59 ng	1360590	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81



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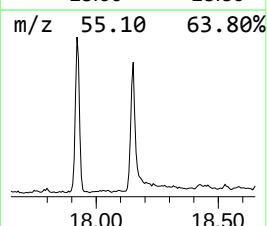
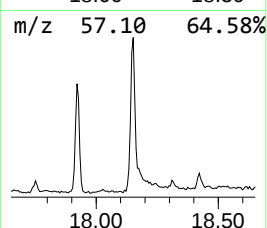
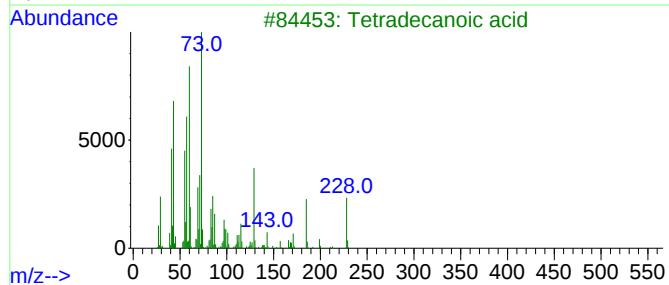
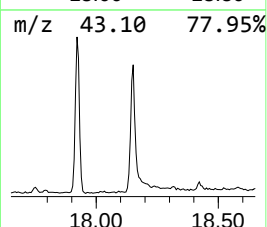
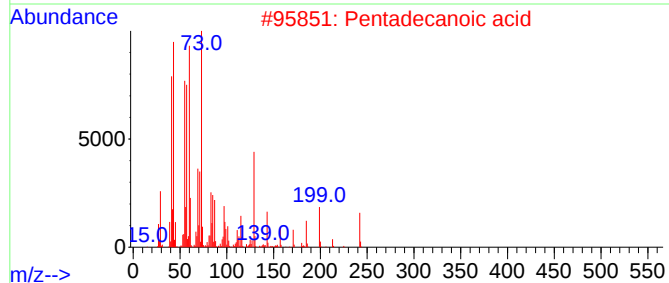
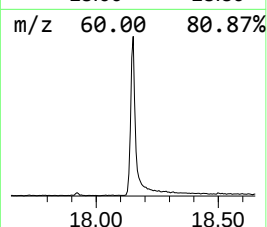
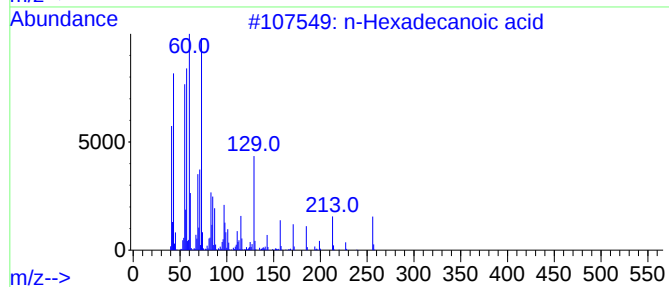
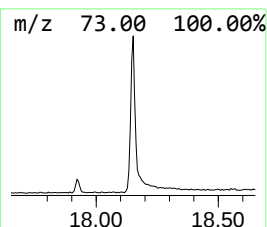
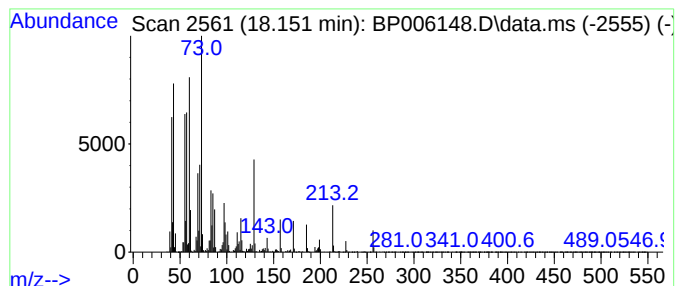
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	12.99 ng	1300480	Phenanthrene-d10	17.257

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		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Undecanoic acid	186	C11H22O2	000112-37-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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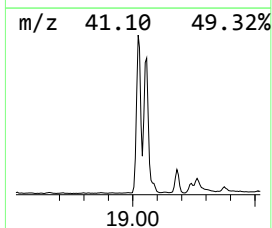
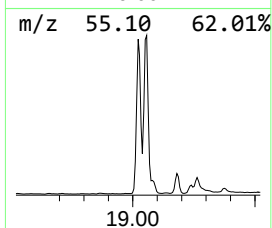
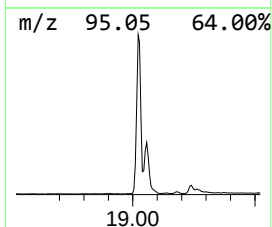
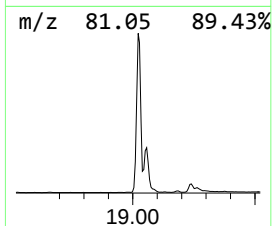
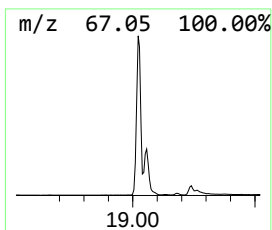
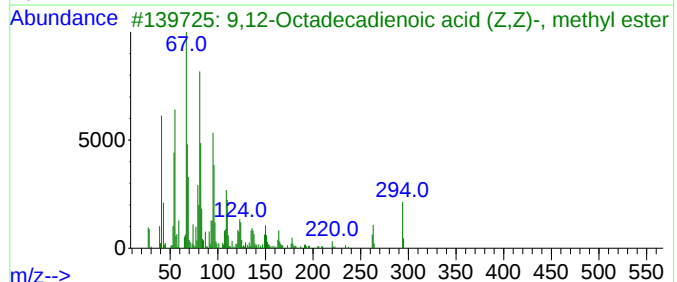
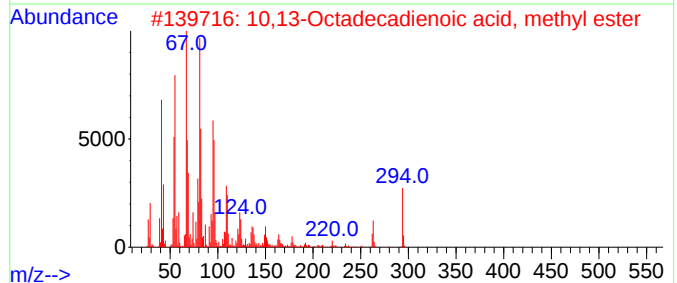
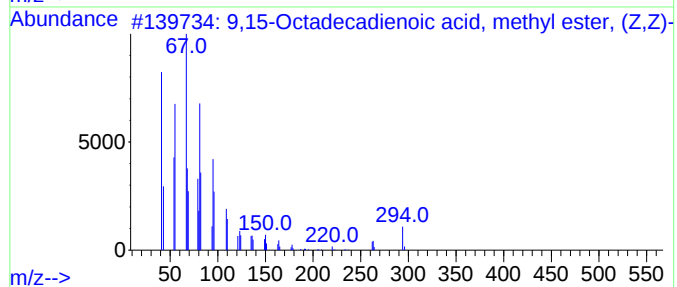
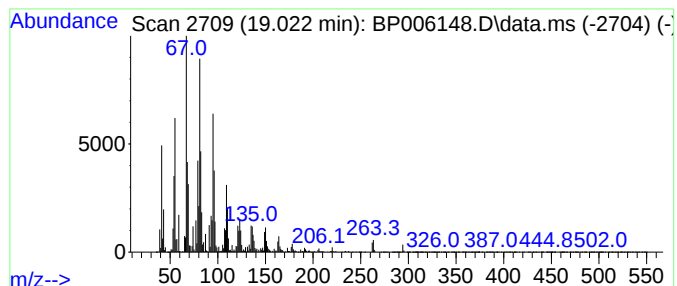
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,15-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.022	95.16 ng	9530100	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
2			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99



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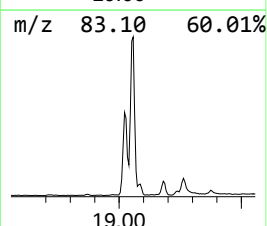
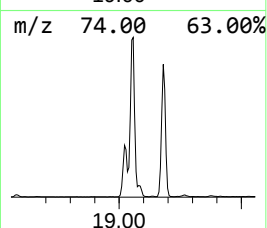
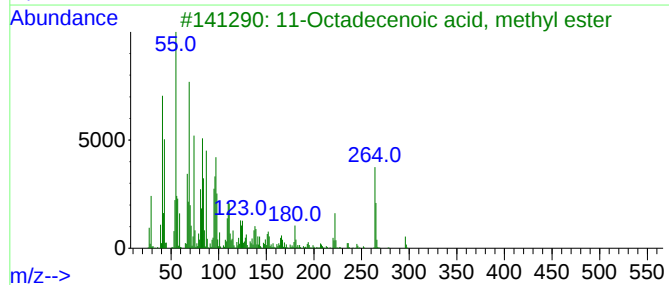
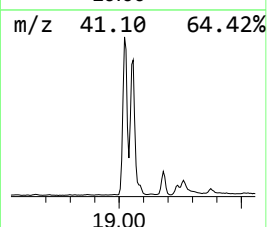
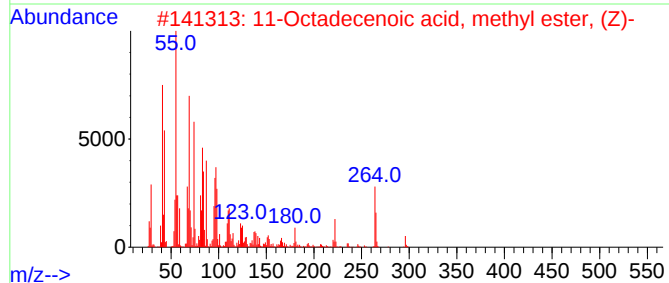
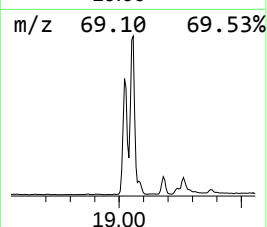
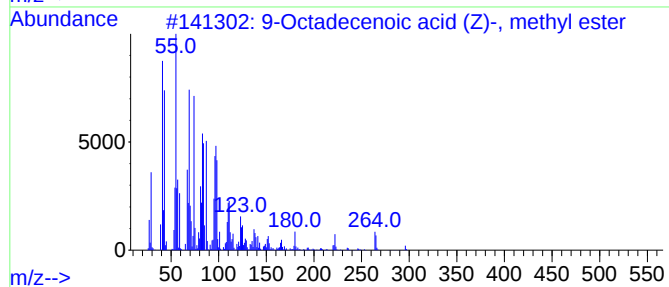
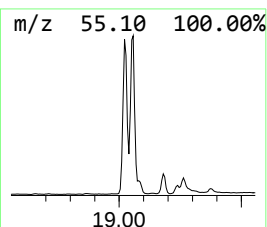
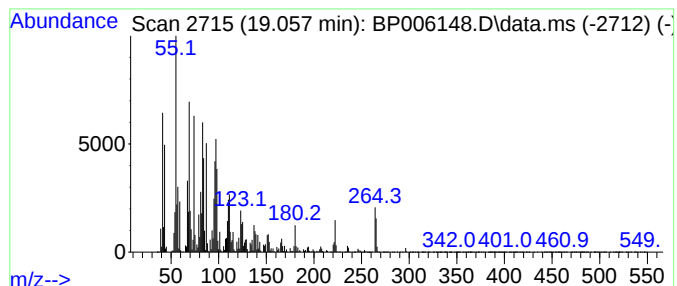
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Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	78.76 ng	7887870	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



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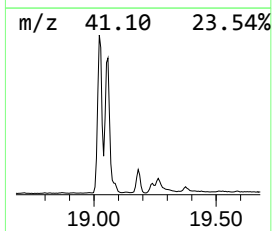
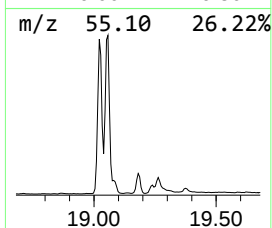
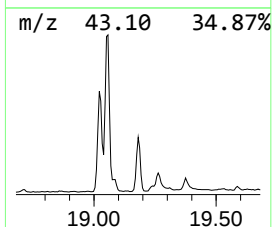
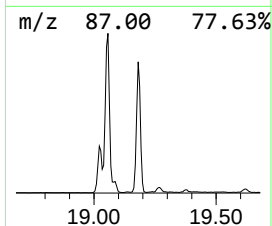
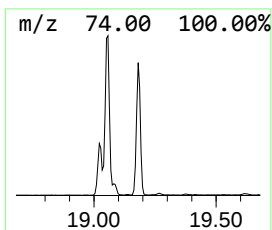
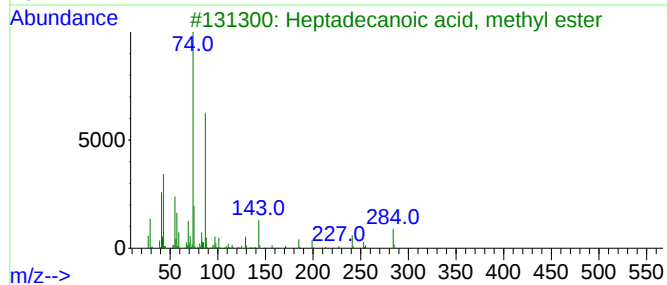
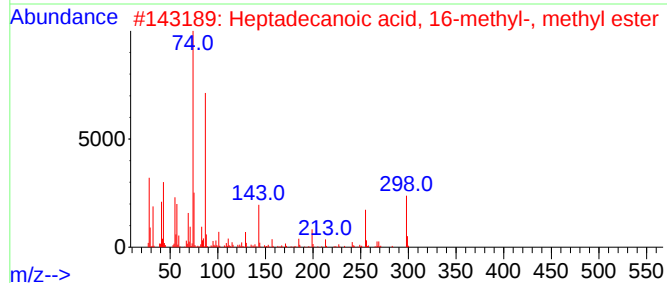
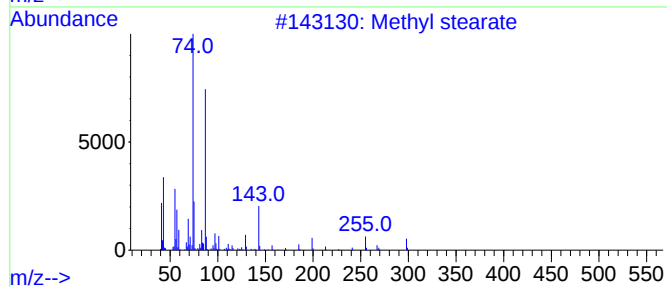
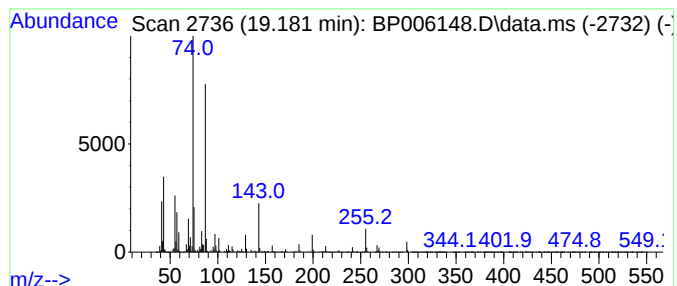
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Peak Number 5 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.181	11.99 ng	1201170	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	99
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86



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BU-03-070621

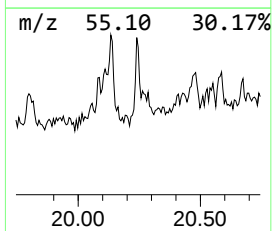
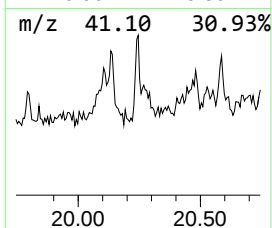
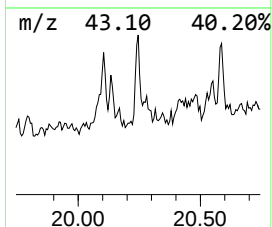
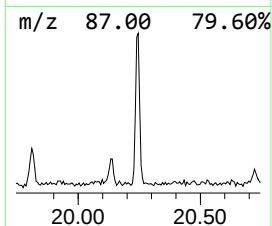
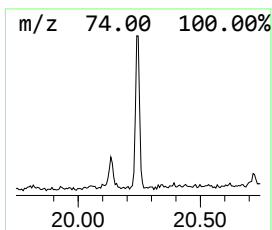
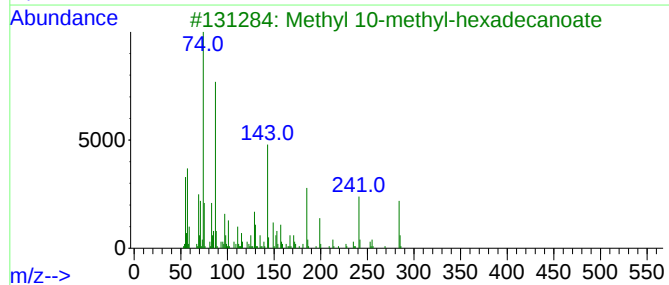
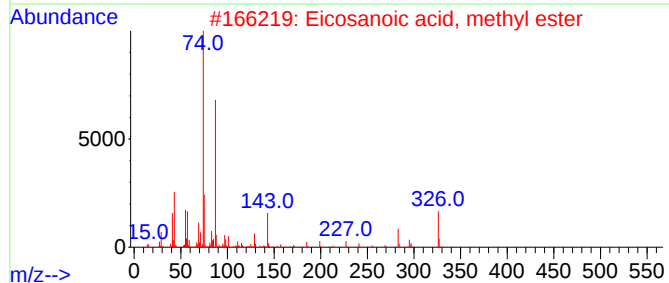
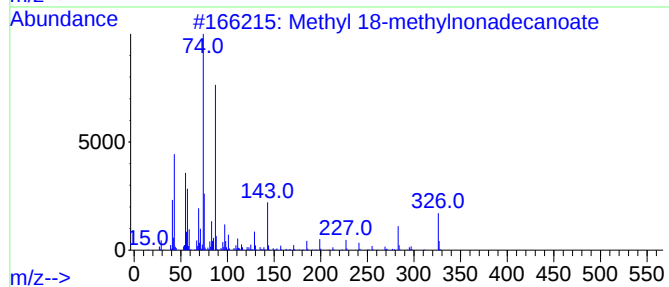
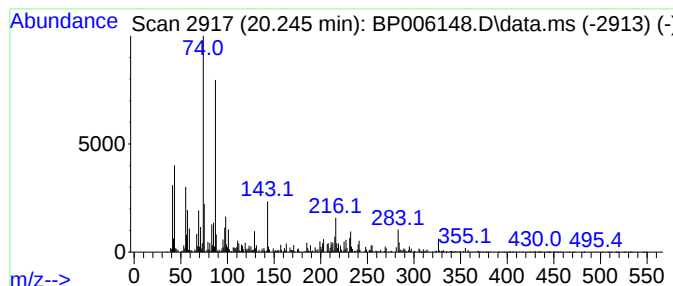
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl 18-methylnonadecanoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.245	4.02 ng	451095	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	93
2			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	91
3			Methyl 10-methyl-hexadecanoate	284	C18H36O2	1000336-50-9	90
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	89
5			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006148.D
Acq On : 08 Jul 2021 19:51
Operator : CG/JU
Sample : M2944-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-070621

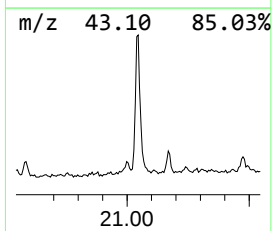
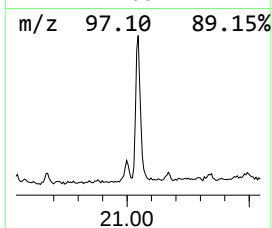
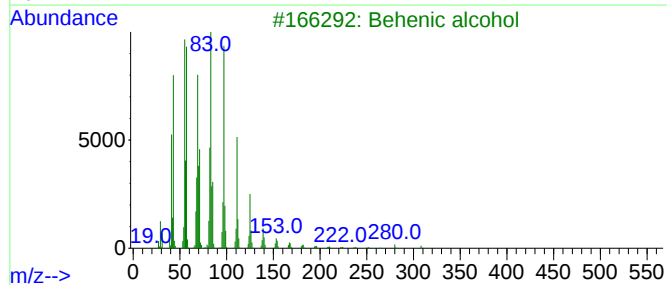
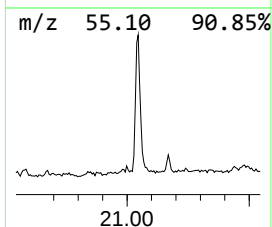
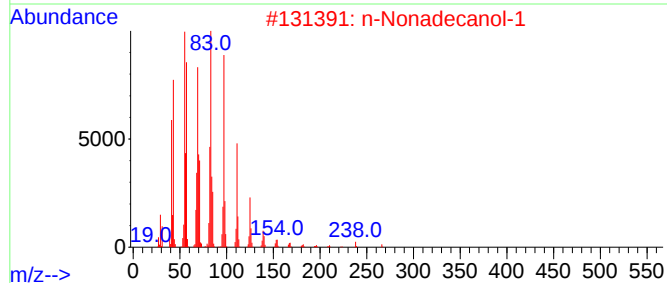
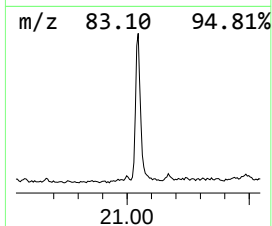
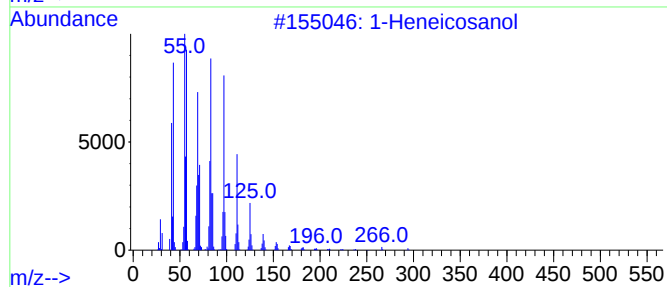
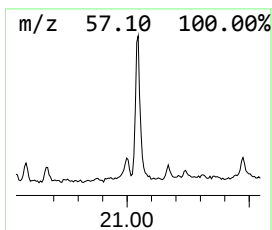
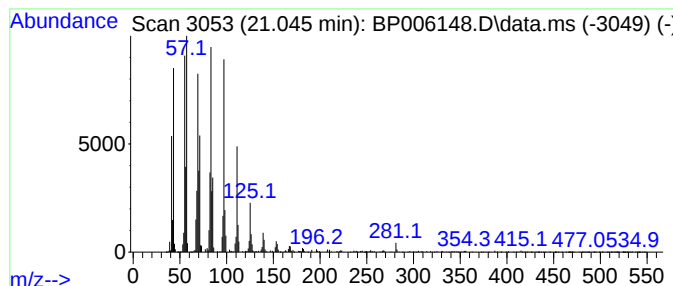
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.045	10.97 ng	1230960	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006148.D
Acq On : 08 Jul 2021 19:51
Operator : CG/JU
Sample : M2944-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-070621

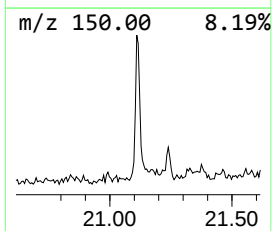
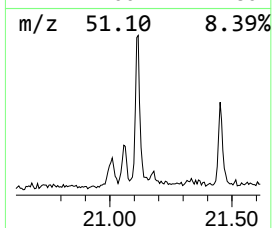
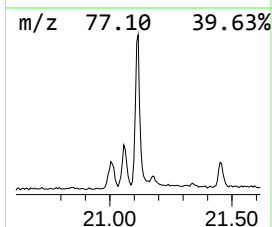
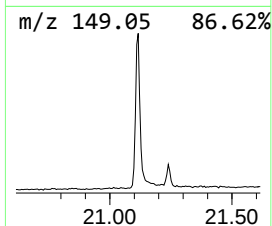
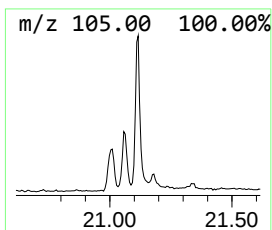
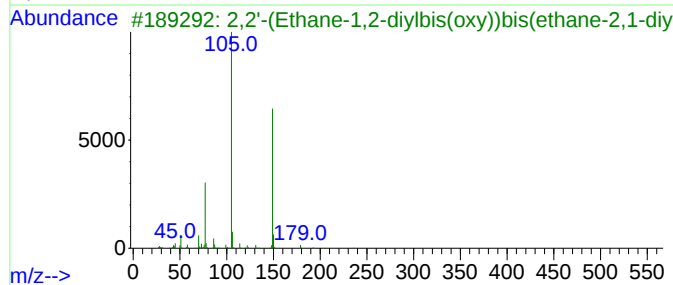
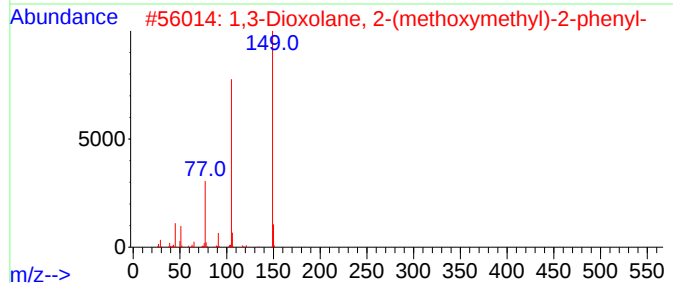
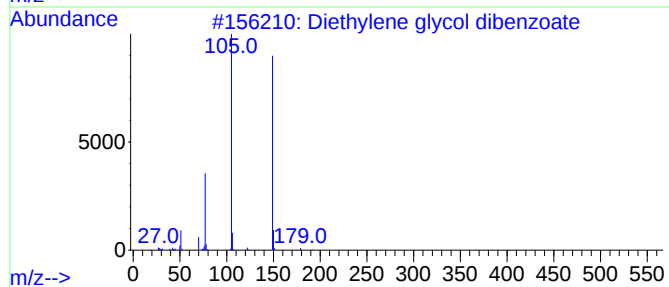
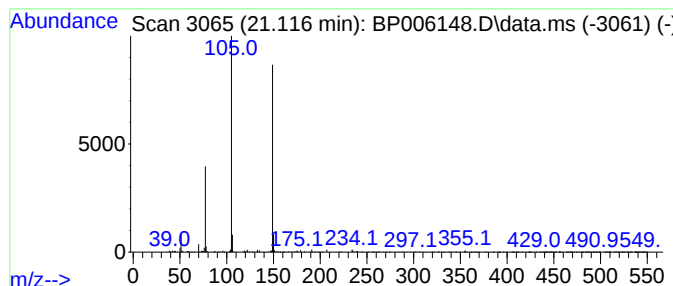
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	4.38 ng	491616	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64
5			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006148.D
Acq On : 08 Jul 2021 19:51
Operator : CG/JU
Sample : M2944-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-070621

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
Hexadecanoic ac...	17.922	13.6	ng	1360590	4	17.257	2002910	20.0
n-Hexadecanoic ...	18.151	13.0	ng	1300480	4	17.257	2002910	20.0
9,15-Octadecadi...	19.022	95.2	ng	9530100	4	17.257	2002910	20.0
9-Octadecenoic ...	19.057	78.8	ng	7887870	4	17.257	2002910	20.0
Methyl stearate	19.181	12.0	ng	1201170	4	17.257	2002910	20.0
Methyl 18-methy...	20.245	4.0	ng	451095	5	21.339	2243350	20.0
1-Heneicosanol	21.045	11.0	ng	1230960	5	21.339	2243350	20.0
Diethylene glyc...	21.116	4.4	ng	491616	5	21.339	2243350	20.0