

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
 Data File : BP008607.D
 Acq On : 30 Dec 2021 13:23
 Operator : CG/JU
 Sample : M5210-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 124027

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-BP122821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.093	14	18	24	rVB	228769	280096	1.13%	0.182%
2	5.469	415	422	434	rBV	6482692	9560043	38.70%	6.223%
3	7.057	684	692	706	rBV	5824442	9671458	39.15%	6.295%
4	7.893	827	834	842	rBV	1745706	2779209	11.25%	1.809%
5	9.046	1020	1030	1042	rBV	3724097	6191113	25.06%	4.030%
6	9.922	1169	1179	1188	rBV	140986	383826	1.55%	0.250%
7	10.693	1302	1310	1316	rBV	2204950	3712904	15.03%	2.417%
8	10.746	1316	1319	1326	rVB	174522	259288	1.05%	0.169%
9	13.151	1721	1728	1741	rVB	10280113	15061631	60.98%	9.804%
10	14.522	1951	1961	1967	rBV	3155431	4665256	18.89%	3.037%
11	14.586	1967	1972	1980	rVB	287918	447066	1.81%	0.291%
12	14.922	2019	2029	2030	rBV	221518	321572	1.30%	0.209%
13	14.945	2030	2033	2040	rVB	264607	402827	1.63%	0.262%
14	15.569	2134	2139	2151	rVB	245712	368032	1.49%	0.240%
15	16.010	2207	2214	2223	rBV	6874472	9821109	39.76%	6.393%
16	17.269	2422	2428	2432	rBV	3425474	4983355	20.18%	3.244%
17	17.310	2432	2435	2441	rVB	748237	1023000	4.14%	0.666%
18	18.057	2557	2562	2568	rBV3	125316	289295	1.17%	0.188%
19	18.175	2576	2582	2603	rBV	8455631	14240820	57.65%	9.270%
20	19.280	2764	2770	2783	rBV2	1247520	3150051	12.75%	2.050%
21	19.410	2785	2792	2819	rVV	14245734	24700516	100.00%	16.078%
22	19.627	2825	2829	2838	rVB2	610689	985578	3.99%	0.642%
23	19.827	2857	2863	2870	rVB	14105654	18113341	73.33%	11.790%
24	20.139	2913	2916	2921	rVB	292003	372857	1.51%	0.243%
25	20.580	2987	2991	2995	rBV	1044269	1145922	4.64%	0.746%
26	20.769	3020	3023	3031	rBV2	449277	563449	2.28%	0.367%
27	21.010	3060	3064	3071	rBV2	725038	1102934	4.47%	0.718%
28	21.069	3071	3074	3079	rBV2	959313	1256230	5.09%	0.818%
29	21.351	3116	3122	3126	rBV	4977154	6856613	27.76%	4.463%
30	22.263	3273	3277	3284	rBV	753817	1361389	5.51%	0.886%
31	23.774	3527	3534	3555	rVB2	3893867	8498988	34.41%	5.532%
32	24.439	3644	3647	3656	rVB2	545827	1057721	4.28%	0.688%

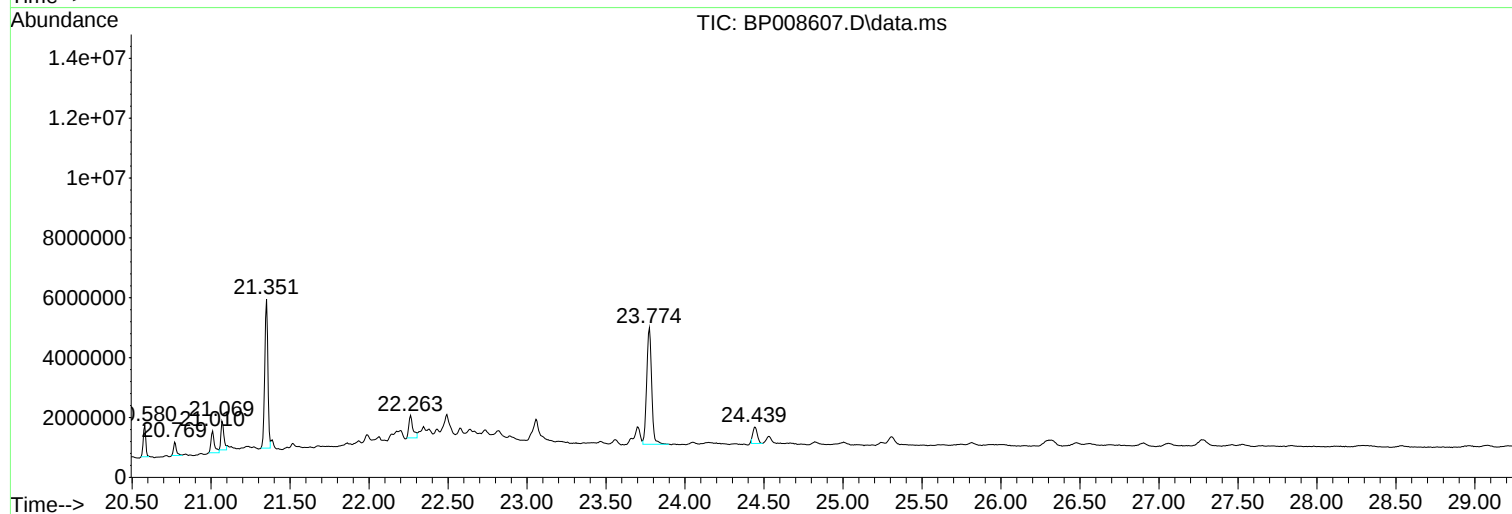
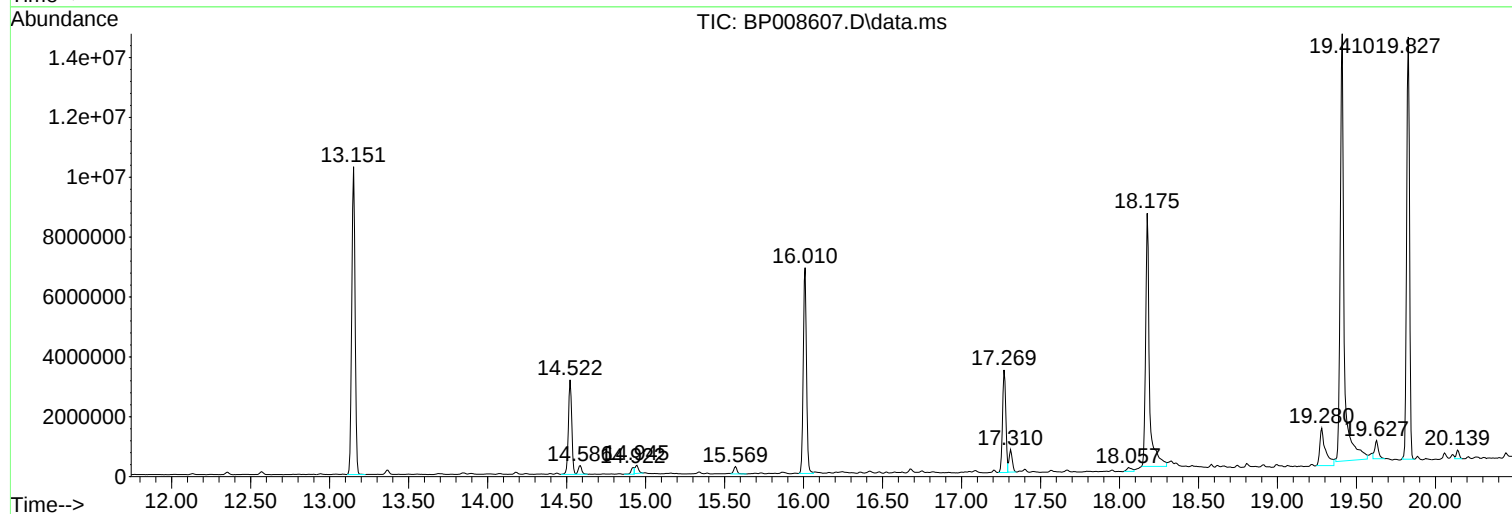
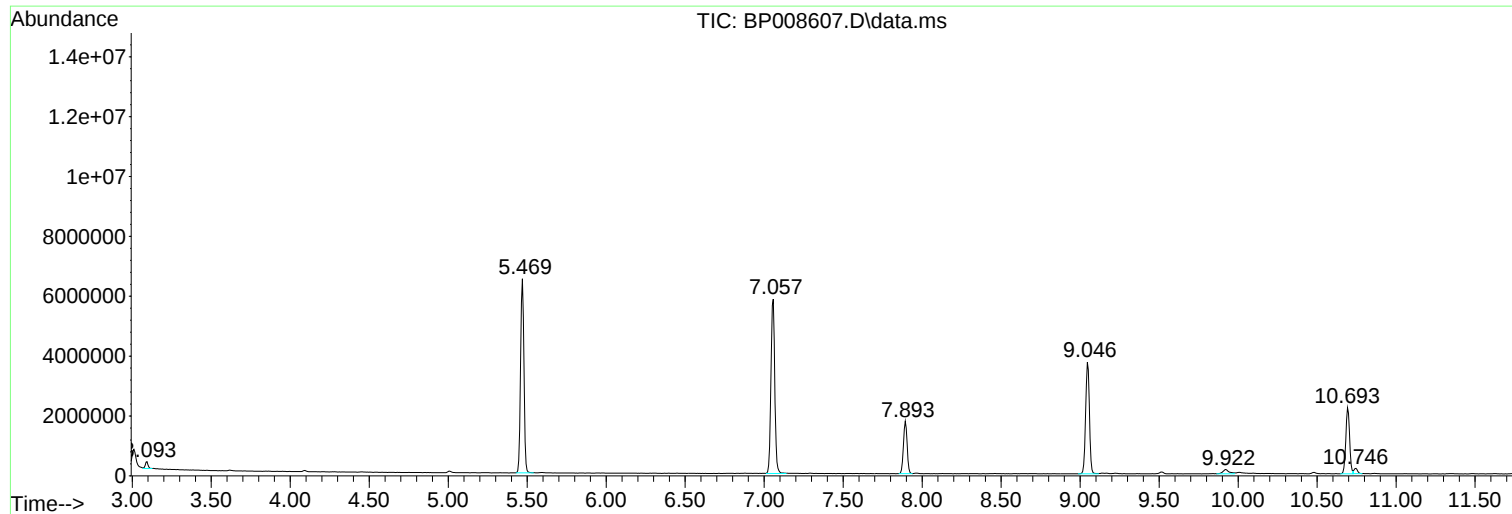
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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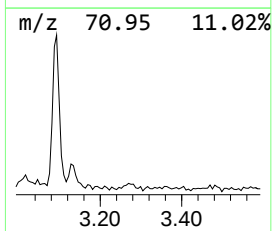
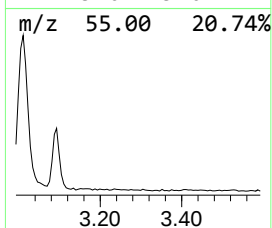
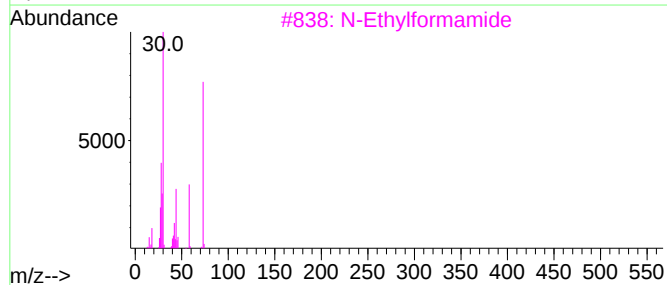
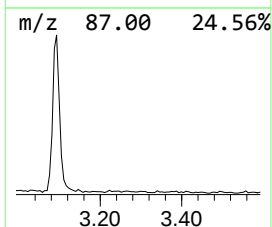
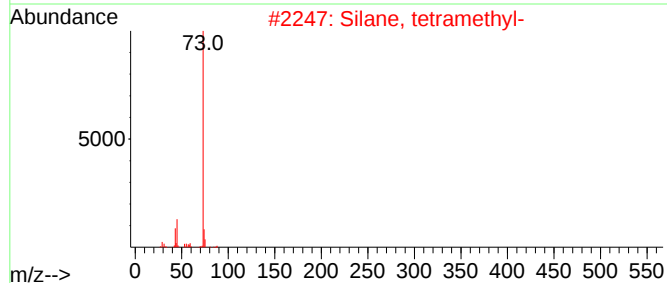
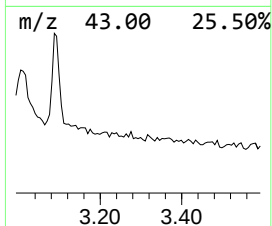
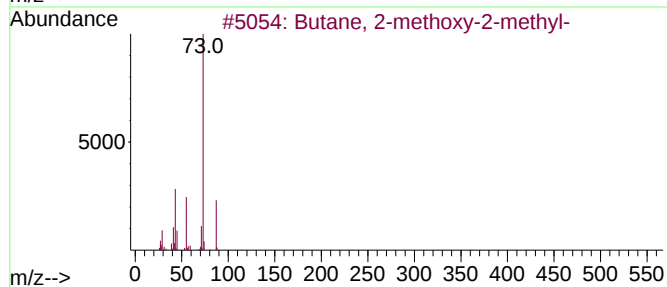
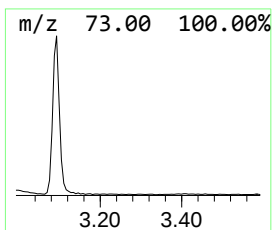
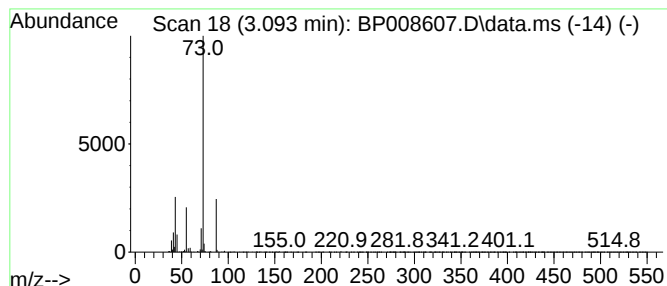
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	2.02 ng	280096	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5			Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	9



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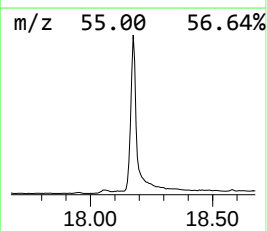
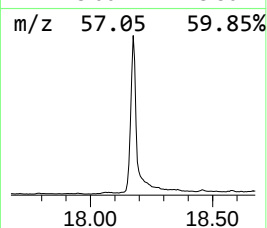
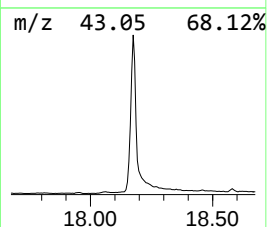
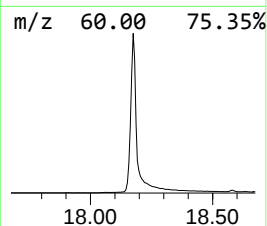
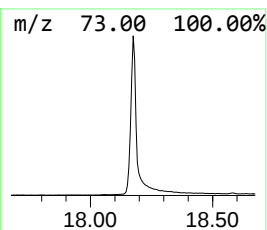
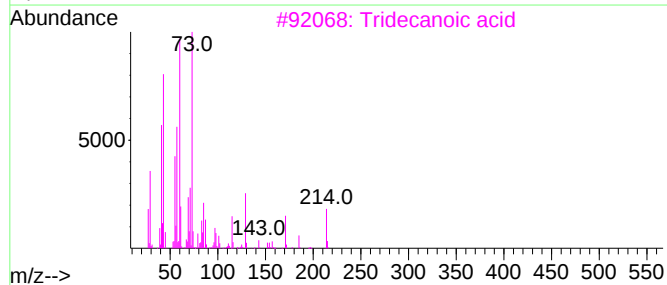
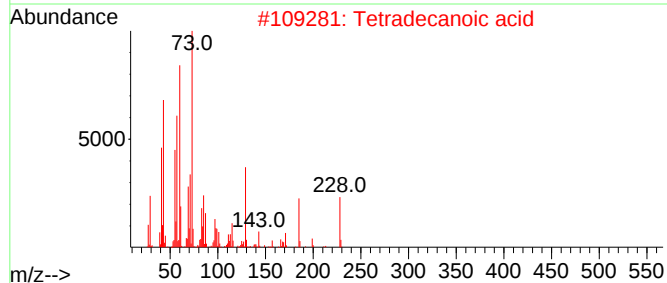
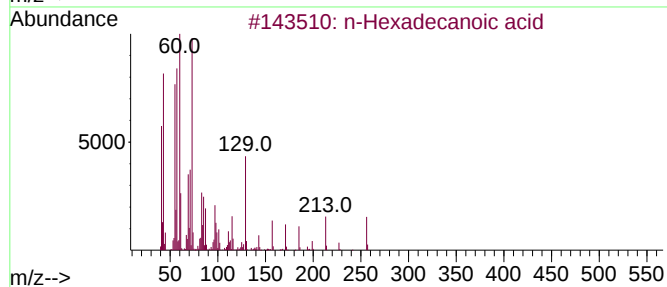
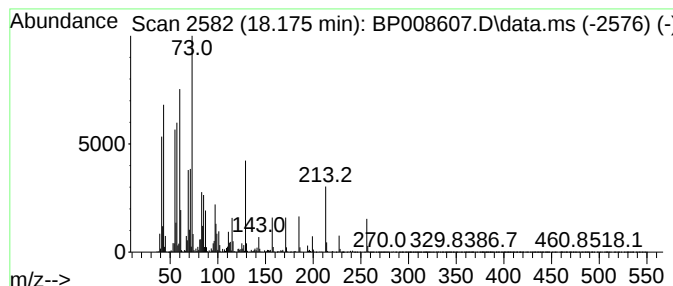
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	57.15 ng	14240800	Phenanthrene-d10	17.269

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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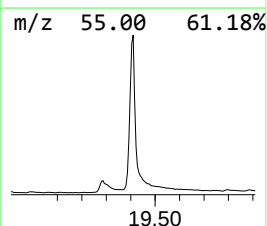
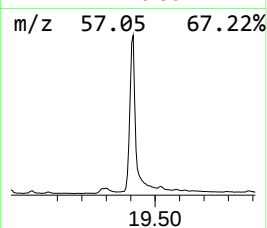
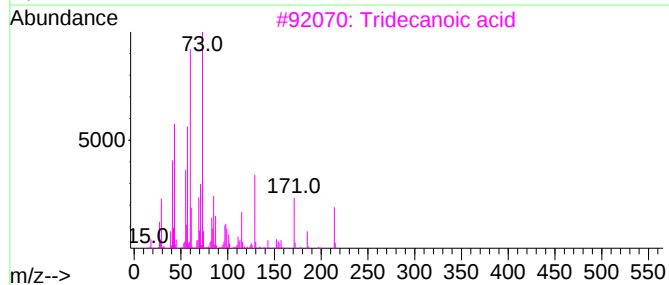
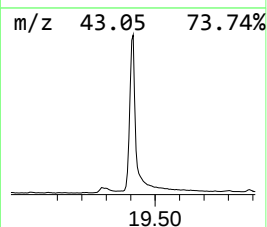
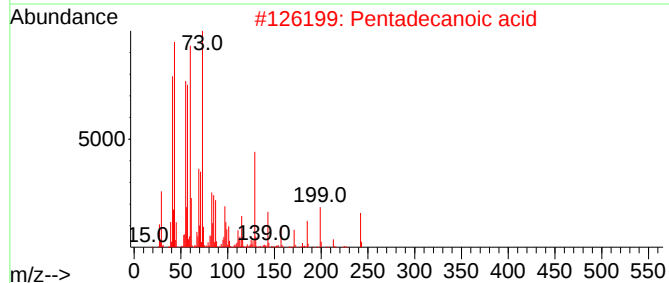
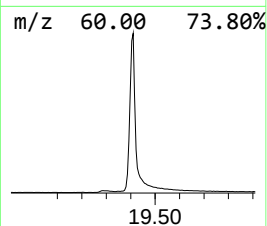
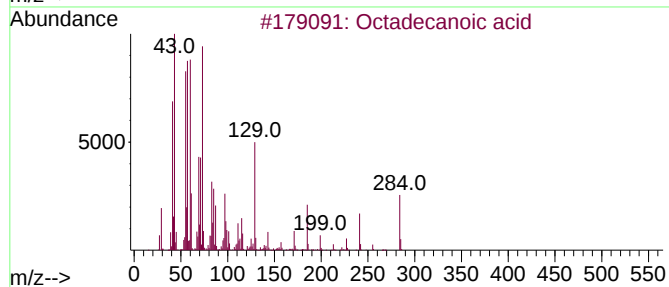
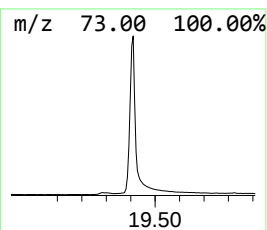
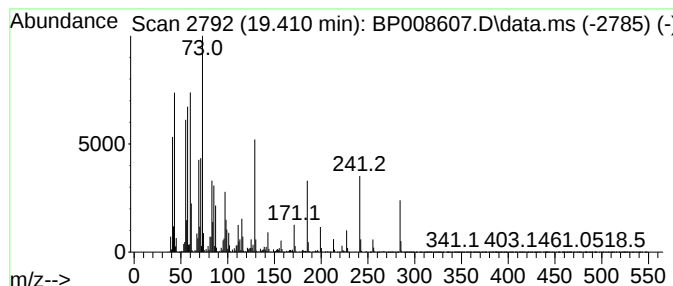
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.410	72.05 ng	24700500	Chrysene-d12	21.351

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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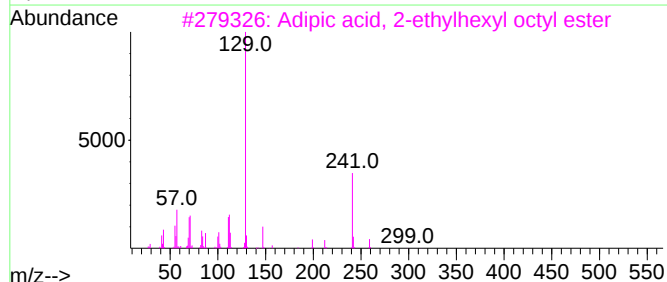
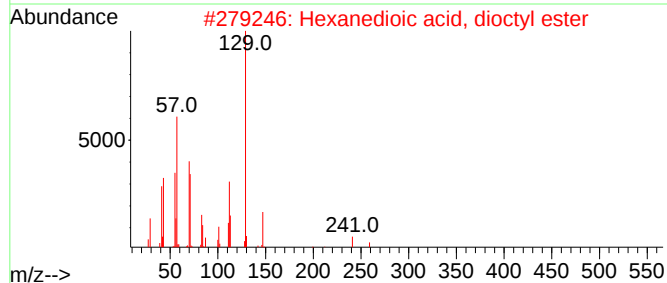
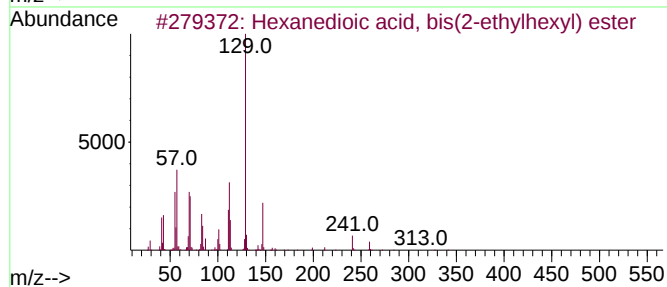
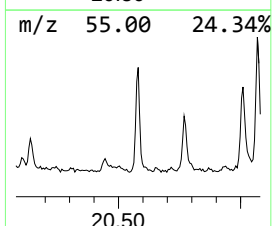
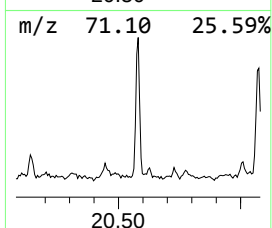
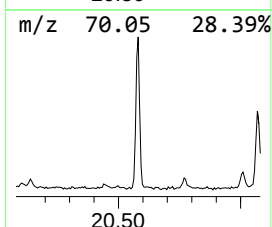
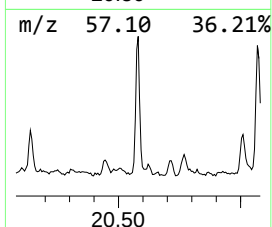
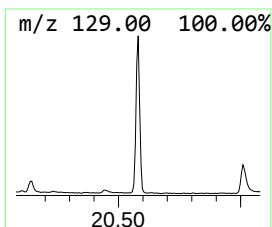
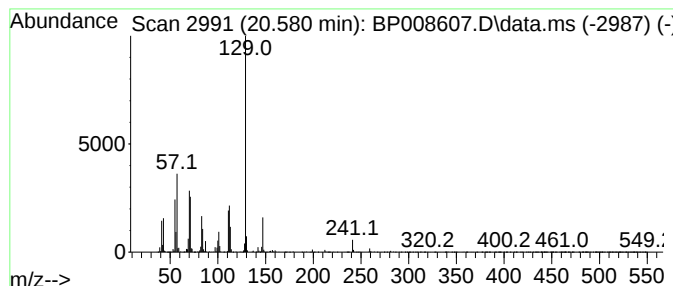
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.580	3.34 ng	1145920	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
3			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
4			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	72
5			Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	58



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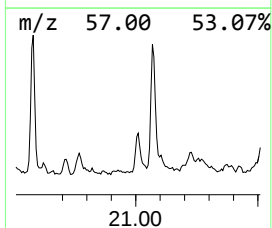
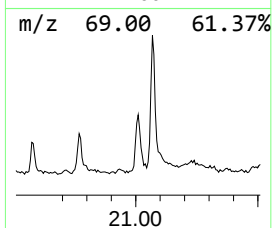
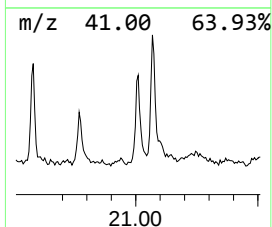
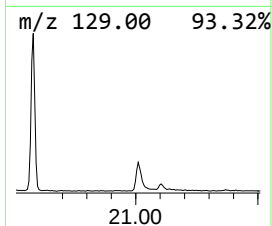
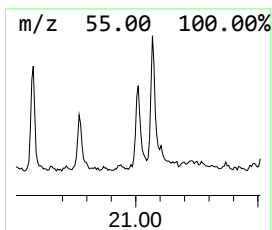
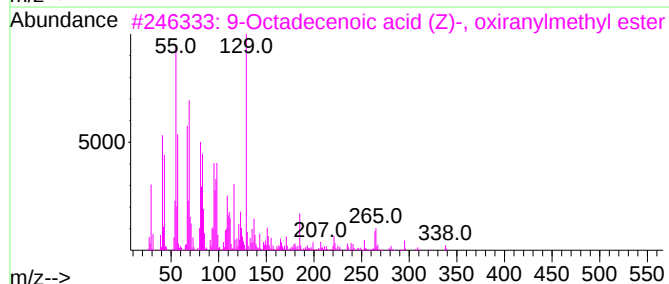
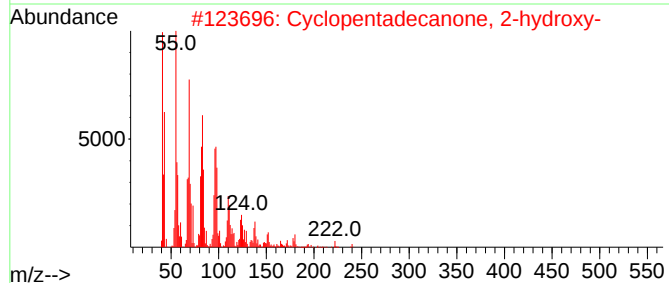
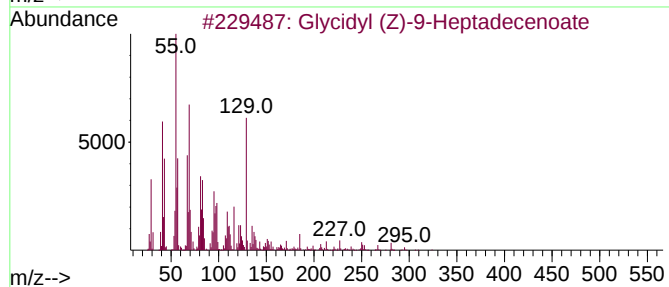
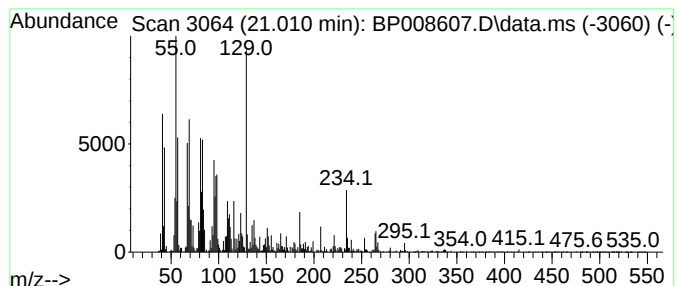
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Peak Number 5 Glycidyl (Z)-9-Heptadecenoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.010	3.22 ng	1102930	Chrysene-d12	21.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycidyl (Z)-9-Heptadecenoate	324	C20H36O3	1000465-63-2	91
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	91
3	9-Octadecenoic acid (Z)-, oxiran...	338	C21H38O3	005431-33-4	87
4	Glycidyl palmitoleate	310	C19H34O3	213738-77-3	87
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	51



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ClientSampleId :
124027

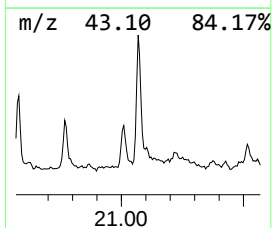
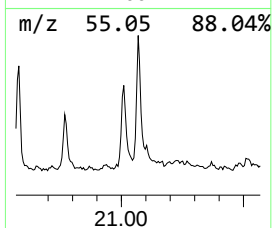
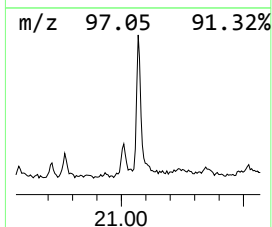
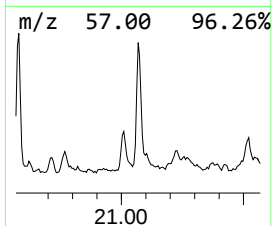
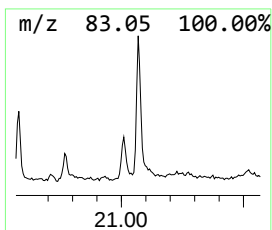
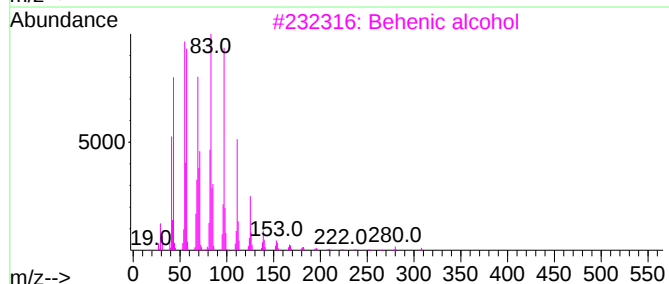
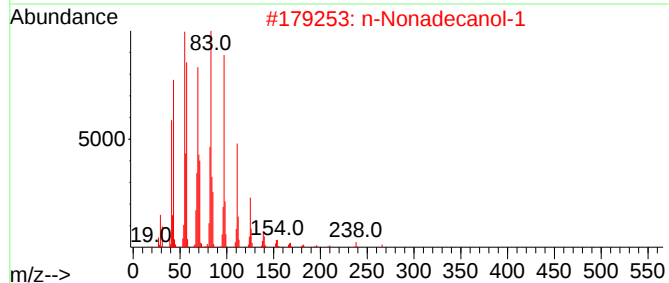
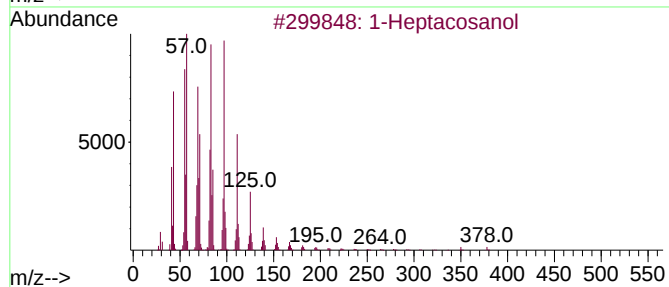
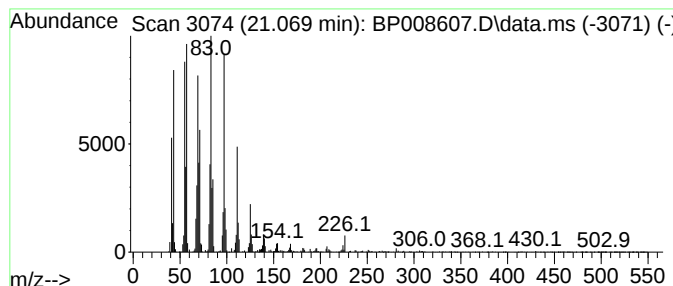
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.069	3.66 ng	1256230	Chrysene-d12	21.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		1-Tetracosene	336	C24H48	010192-32-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008607.D
Acq On : 30 Dec 2021 13:23
Operator : CG/JU
Sample : M5210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
124027

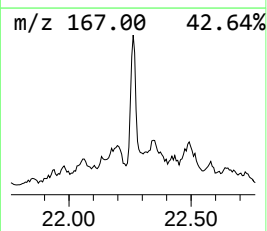
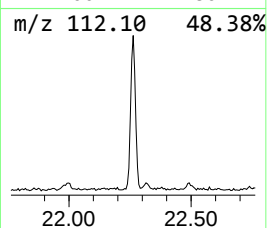
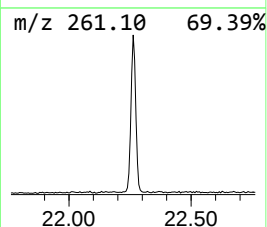
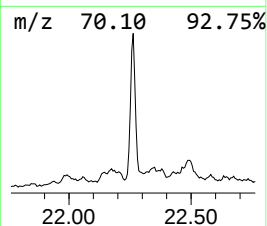
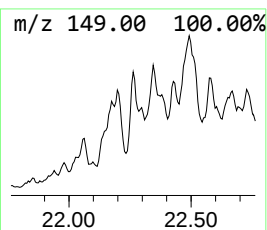
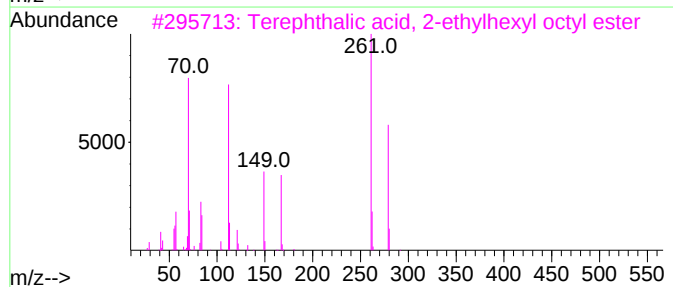
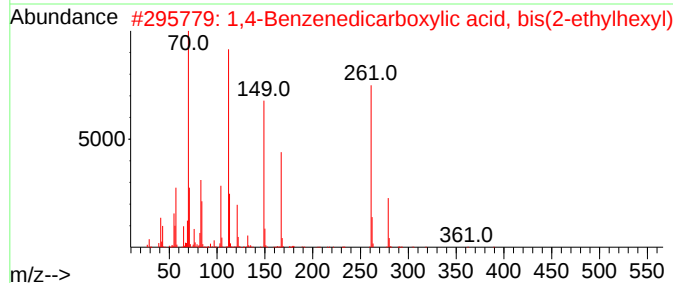
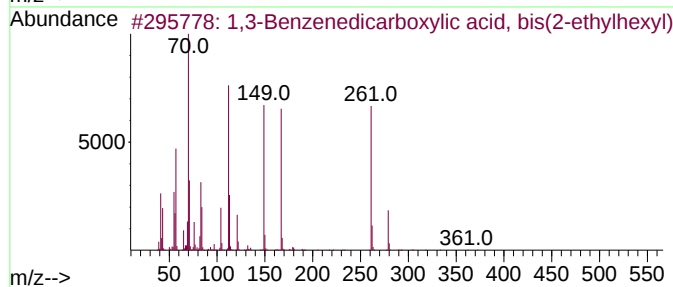
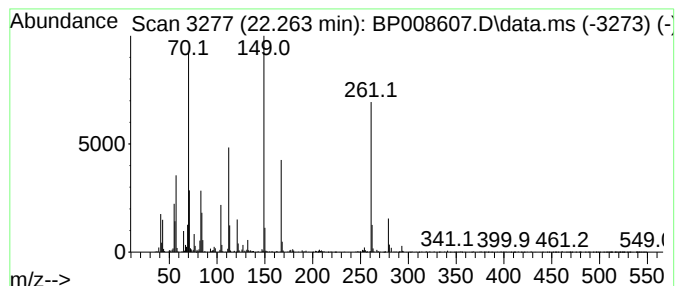
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.263	3.97 ng	1361390	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	74
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	52
4			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	50
5			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008607.D
Acq On : 30 Dec 2021 13:23
Operator : CG/JU
Sample : M5210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
124027

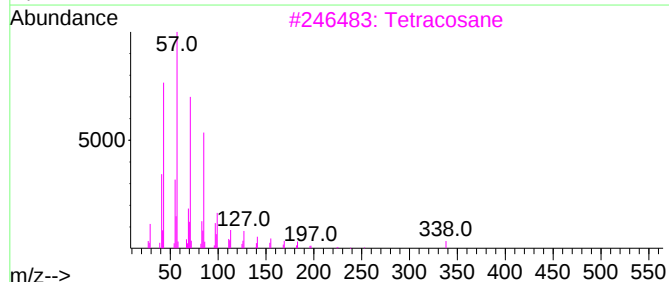
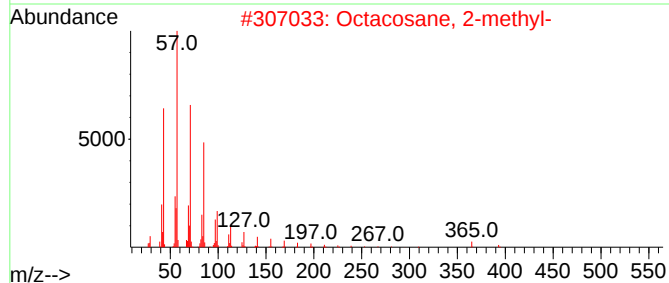
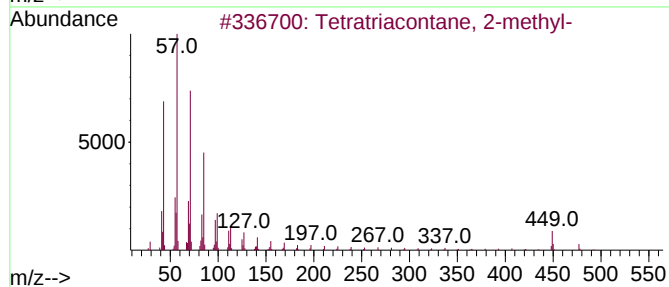
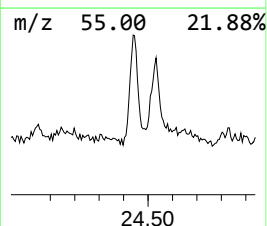
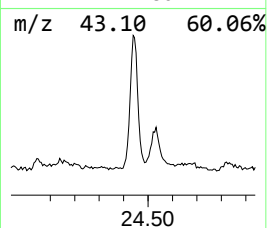
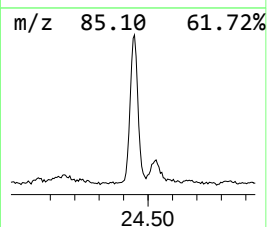
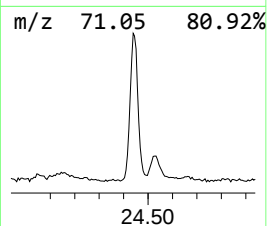
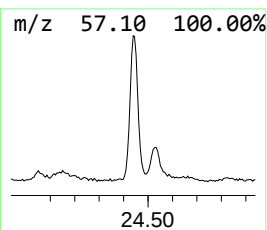
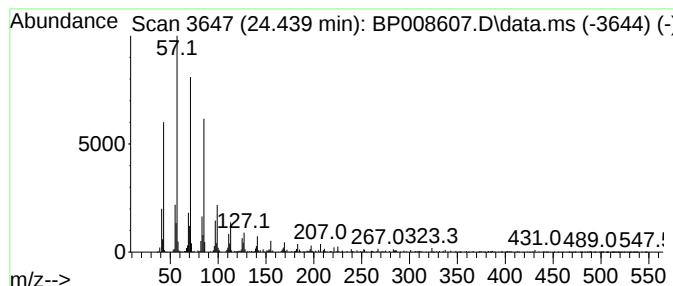
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratriacontane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.439	2.49 ng	1057720	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Triacotane, 1-iodo-	548	C30H61I	1000406-32-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008607.D
Acq On : 30 Dec 2021 13:23
Operator : CG/JU
Sample : M5210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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...	3.093	2.0	ng	280096	1	7.893	2779210	20.0
n-Hexadecanoic ...	18.174	57.1	ng	14240800	4	17.269	4983360	20.0
Octadecanoic acid	19.410	72.0	ng	24700500	5	21.351	6856610	20.0
Hexanedioic aci...	20.580	3.3	ng	1145920	5	21.351	6856610	20.0
Glycidyl (Z)-9-...	21.010	3.2	ng	1102930	5	21.351	6856610	20.0
1-Heptacosanol	21.069	3.7	ng	1256230	5	21.351	6856610	20.0
1,3-Benzenedica...	22.263	4.0	ng	1361390	5	21.351	6856610	20.0
Tetratriacontan...	24.439	2.5	ng	1057720	6	23.774	8498990	20.0