

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
 Data File : BP006186.D
 Acq On : 12 Jul 2021 17:56
 Operator : CG/JU
 Sample : M3002-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-F

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: BP006186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	316	320	327	rVB	49041	73525	1.44%	0.174%
2	5.440	391	400	420	rBV	2374897	3725929	73.04%	8.811%
3	7.052	667	674	692	rBV	2167359	3819512	74.87%	9.032%
4	7.857	804	811	819	rBV	644458	1055747	20.70%	2.497%
5	9.028	1003	1010	1029	rBV	1365526	2377078	46.60%	5.621%
6	10.451	1245	1252	1278	rBV	979743	2025646	39.71%	4.790%
7	10.663	1280	1288	1301	rVV	863910	1489090	29.19%	3.521%
8	13.122	1699	1706	1719	rBV	2909016	4328394	84.85%	10.236%
9	13.398	1743	1753	1760	rBV	387034	620614	12.17%	1.468%
10	13.710	1802	1806	1815	rBV	44775	73966	1.45%	0.175%
11	14.151	1877	1881	1887	rBV5	25588	53786	1.05%	0.127%
12	14.392	1916	1922	1929	rBV4	34315	90830	1.78%	0.215%
13	14.498	1933	1940	1946	rBV	1233658	1863398	36.53%	4.406%
14	14.910	2004	2010	2017	rBV3	49557	116716	2.29%	0.276%
15	15.287	2069	2074	2077	rBV	71215	117493	2.30%	0.278%
16	15.316	2077	2079	2086	rVB	77939	118031	2.31%	0.279%
17	15.475	2102	2106	2116	rVB3	101422	166478	3.26%	0.394%
18	15.992	2183	2194	2202	rBV	2612962	4045562	79.30%	9.567%
19	16.457	2269	2273	2277	rBV	54000	87076	1.71%	0.206%
20	16.969	2356	2360	2364	rBV2	36768	55040	1.08%	0.130%
21	17.245	2401	2407	2412	rBV	1418671	2015172	39.50%	4.765%
22	17.904	2515	2519	2530	rVB	266719	350509	6.87%	0.829%
23	18.128	2553	2557	2566	rBV	765412	1136133	22.27%	2.687%
24	18.404	2601	2604	2613	rBV6	36500	78336	1.54%	0.185%
25	18.957	2695	2698	2702	rVB3	53654	66081	1.30%	0.156%
26	19.004	2703	2706	2708	rBV2	85190	101937	2.00%	0.241%
27	19.033	2708	2711	2715	rVB	544534	578078	11.33%	1.367%
28	19.163	2729	2733	2739	rBV	224356	251330	4.93%	0.594%
29	19.257	2745	2749	2752	rBV2	148899	236108	4.63%	0.558%
30	19.357	2763	2766	2775	rVB	290842	389758	7.64%	0.922%
31	19.798	2835	2841	2846	rBV	4087307	5101315	100.00%	12.063%
32	20.063	2883	2886	2893	rBV3	97022	169383	3.32%	0.401%
33	20.410	2942	2945	2949	rBV2	149459	158835	3.11%	0.376%
34	21.021	3045	3049	3055	rBV2	558717	888763	17.42%	2.102%
35	21.321	3096	3100	3105	rBV	1691269	2073900	40.65%	4.904%
36	23.704	3499	3505	3520	rVB2	1160584	2388347	46.82%	5.648%

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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

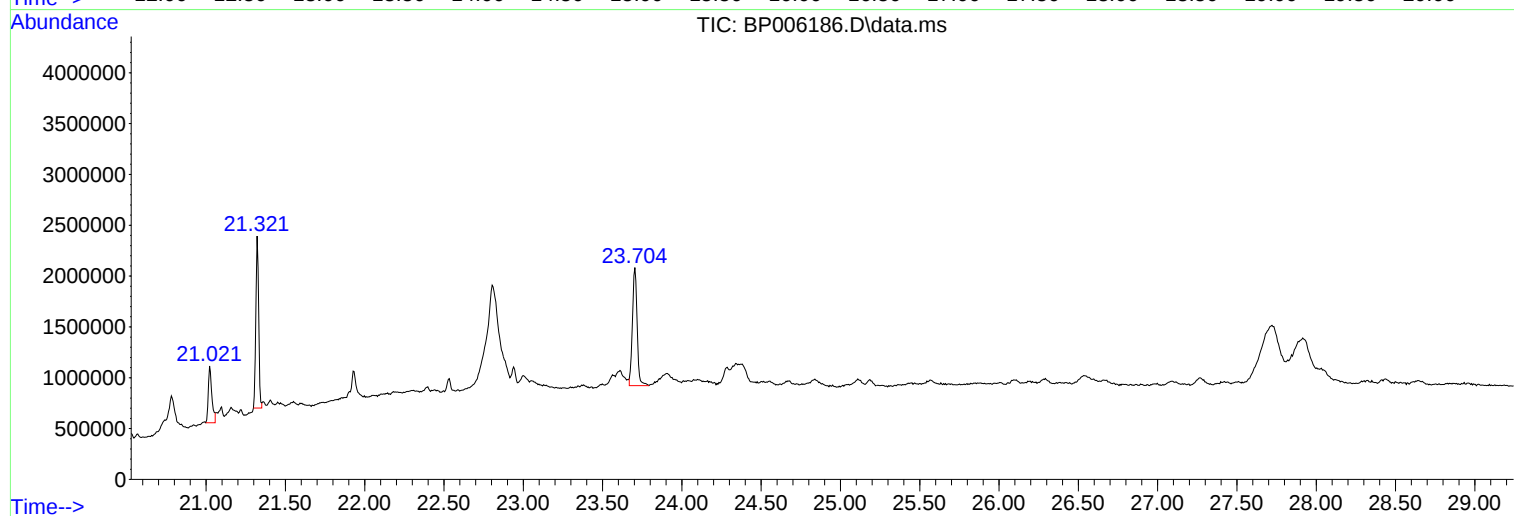
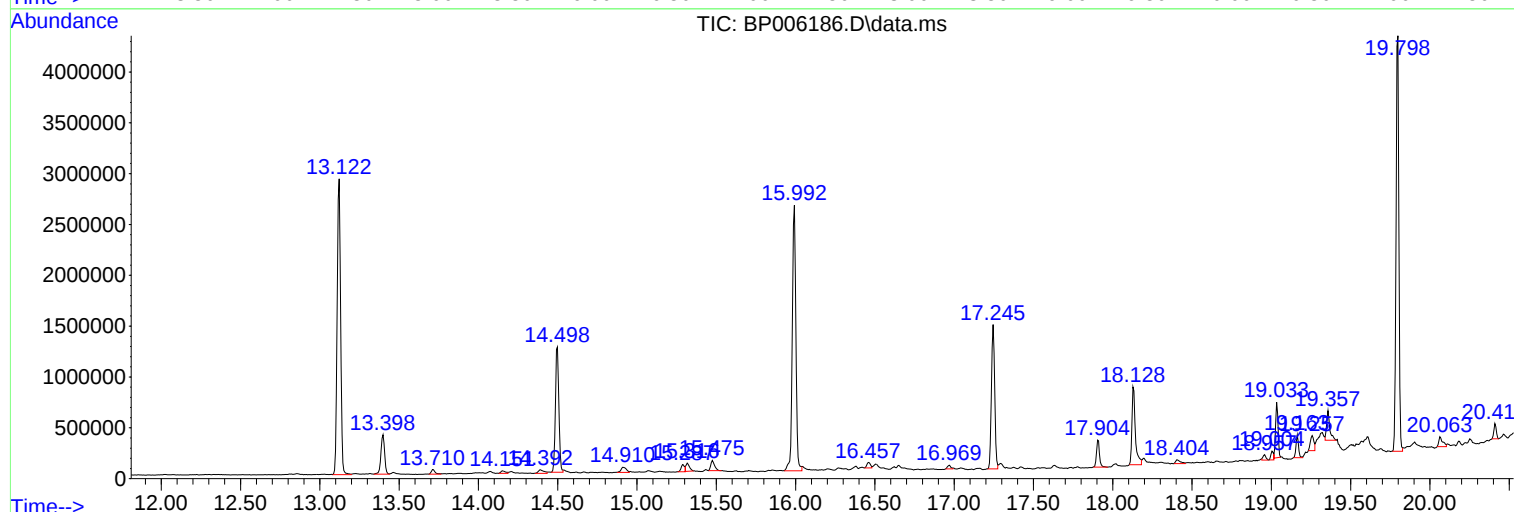
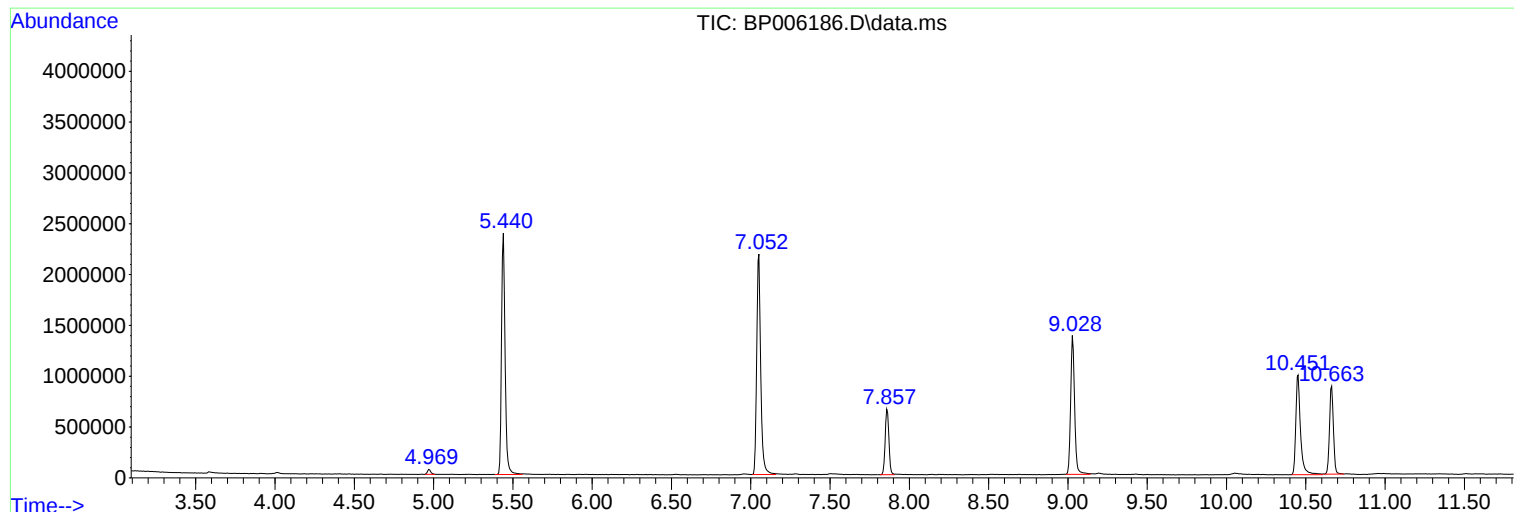
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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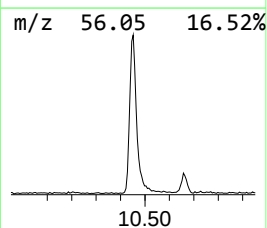
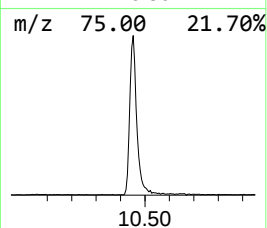
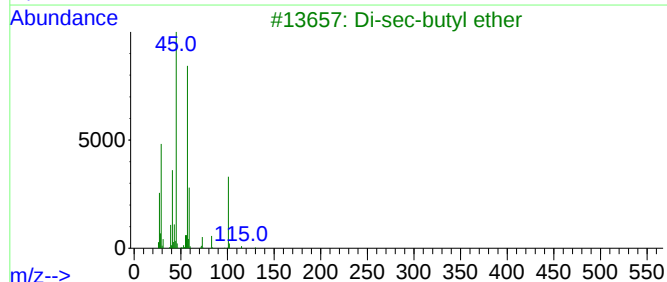
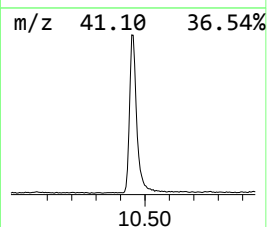
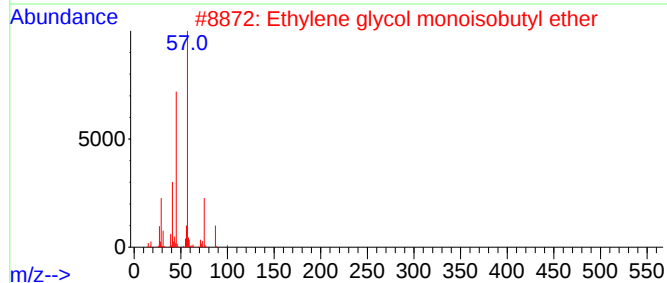
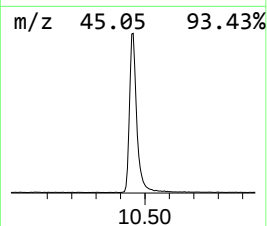
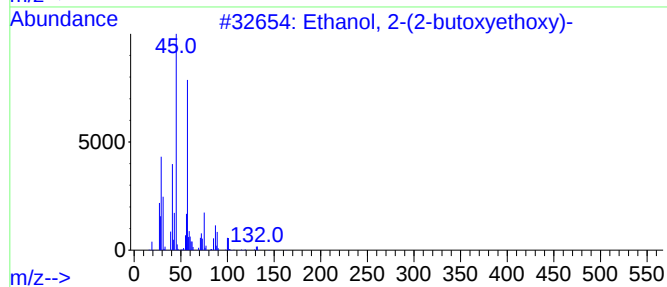
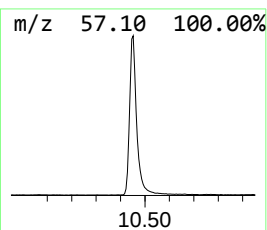
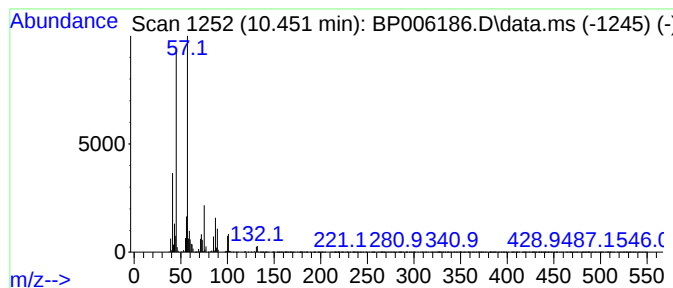
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	27.21 ng	2025650	Naphthalene-d8	10.663

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			Di-sec-butyl ether	130	C8H18O	006863-58-7	50
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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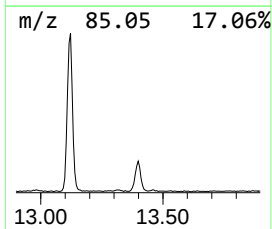
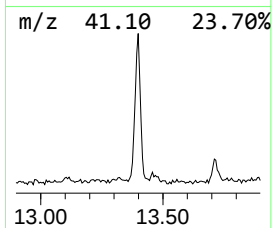
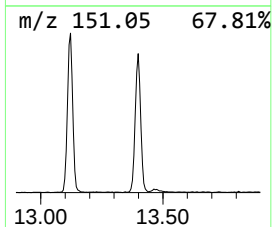
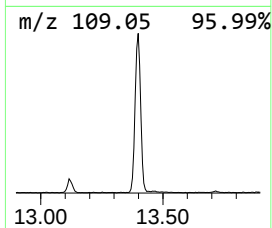
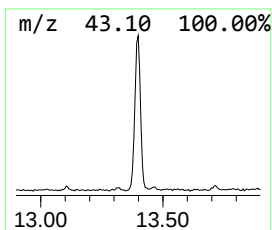
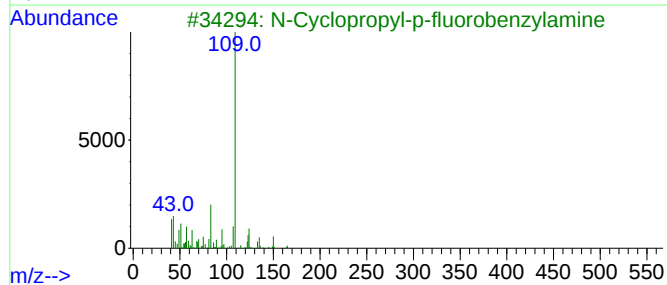
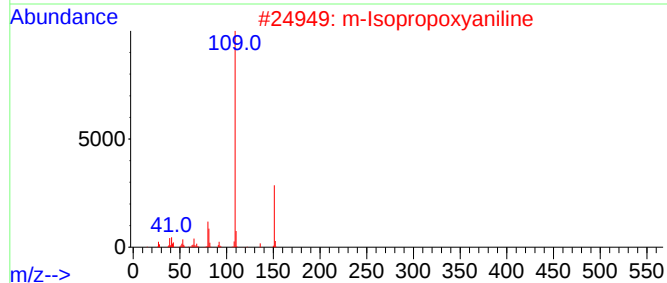
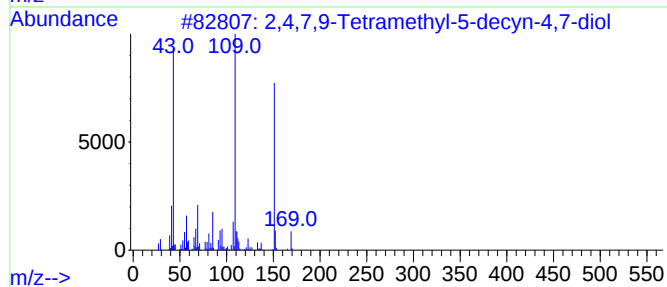
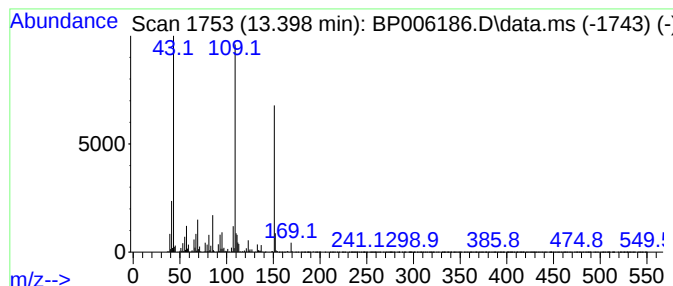
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	6.66 ng	620614	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53		
3	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	49		
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	42		
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42		



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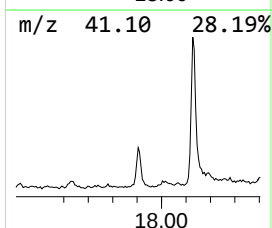
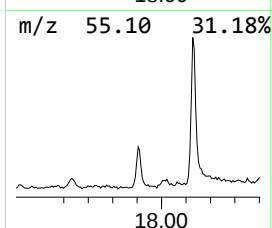
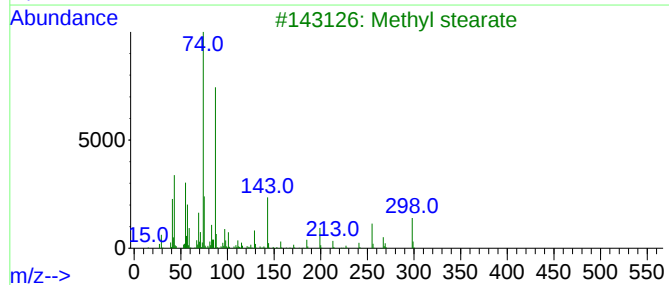
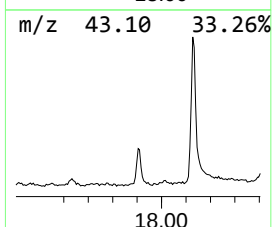
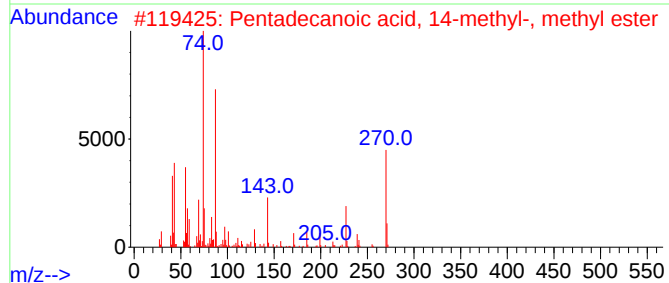
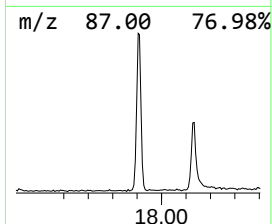
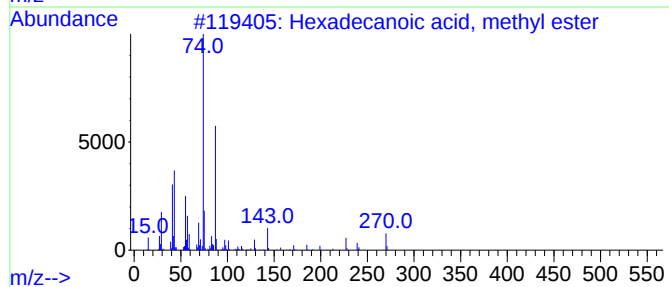
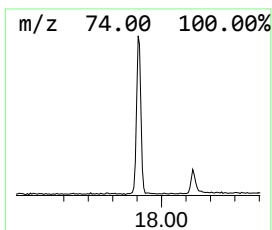
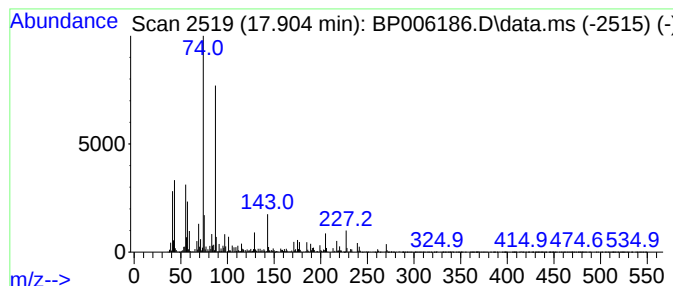
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.904	3.48 ng	350509	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl stearate	298	C19H38O2	000112-61-8	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80



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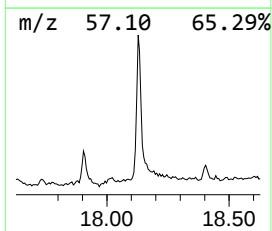
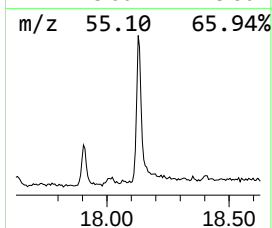
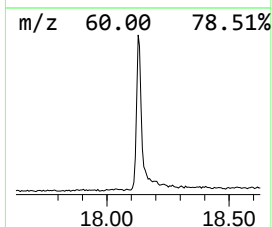
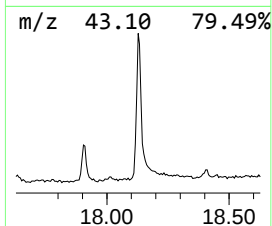
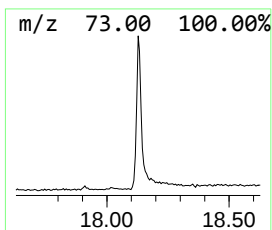
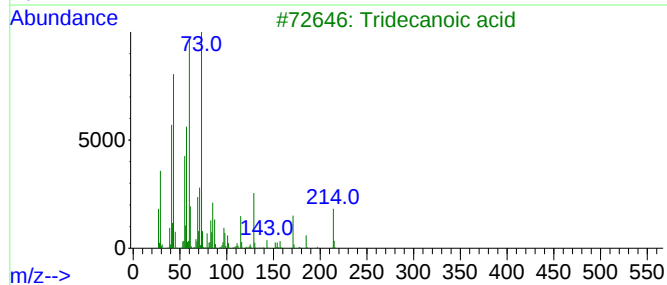
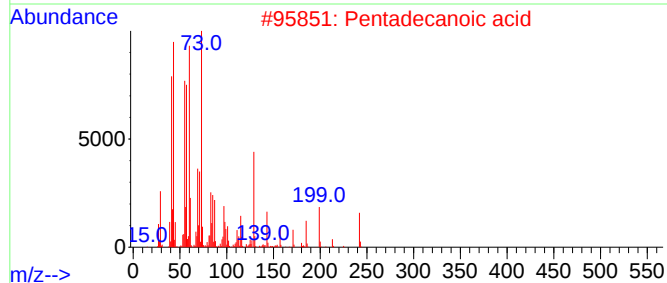
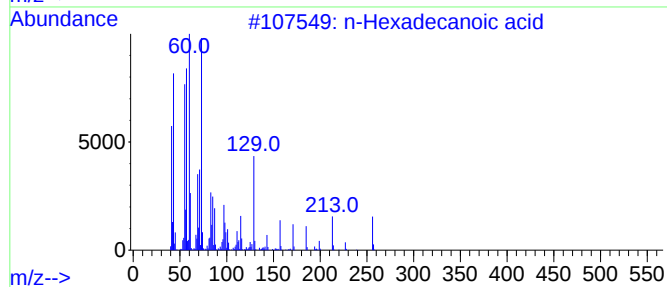
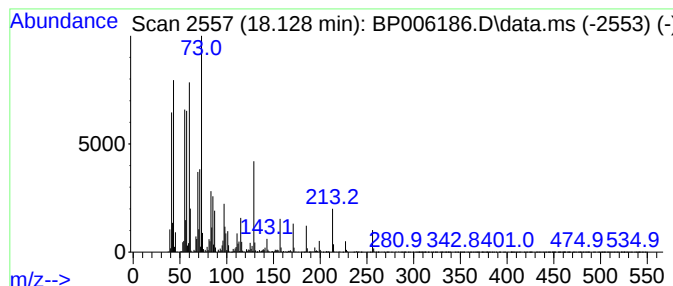
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.128	11.28 ng	1136130	Phenanthrene-d10	17.245

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			Undecanoic acid	186	C11H22O2	000112-37-8	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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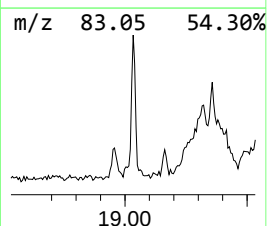
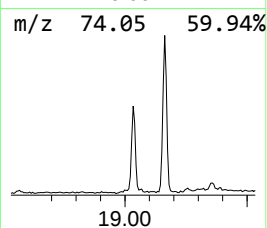
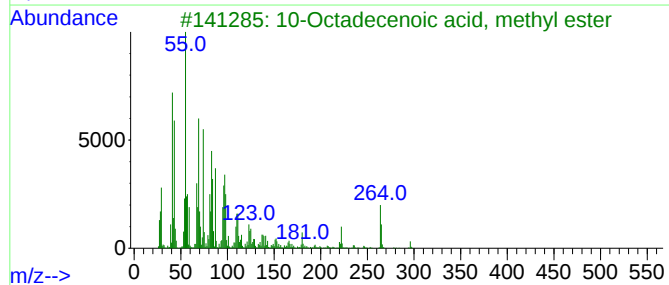
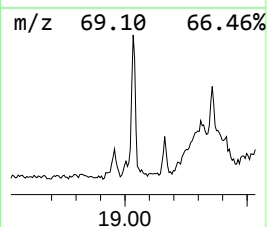
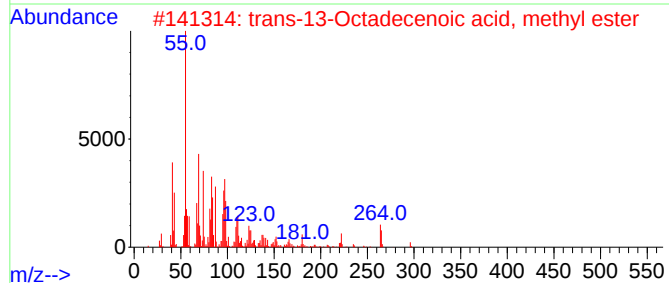
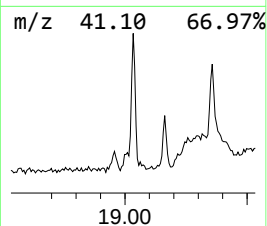
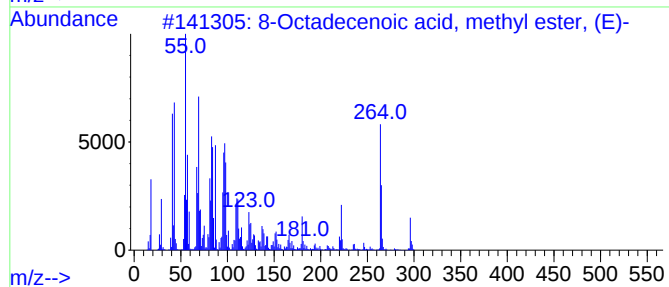
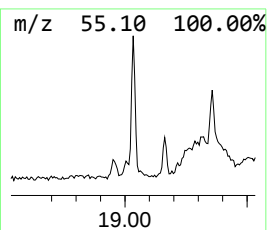
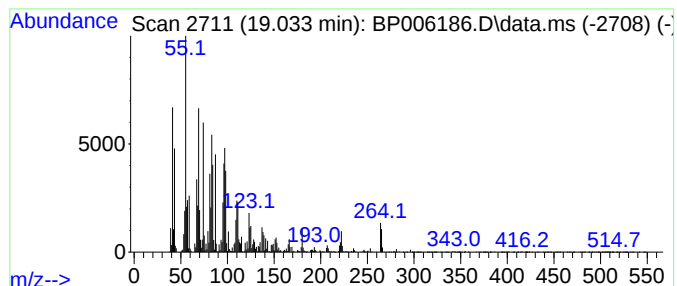
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 8-Octadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.033	5.74 ng	578078	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
5			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006186.D
Acq On : 12 Jul 2021 17:56
Operator : CG/JU
Sample : M3002-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-F

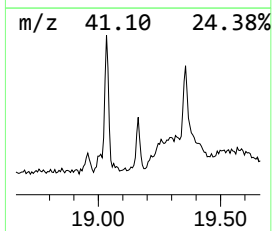
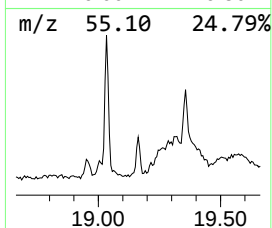
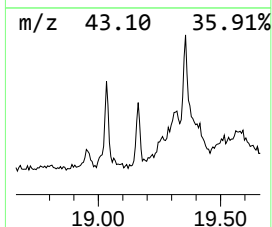
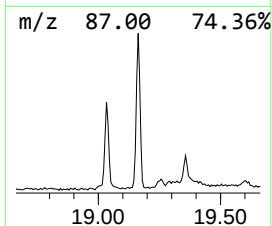
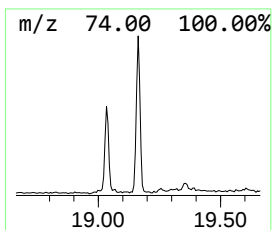
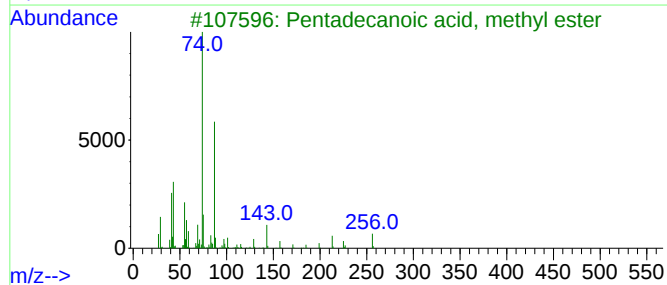
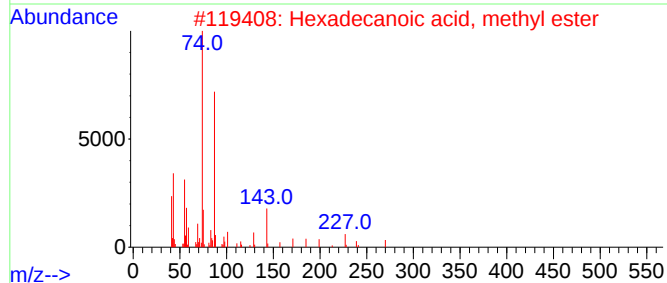
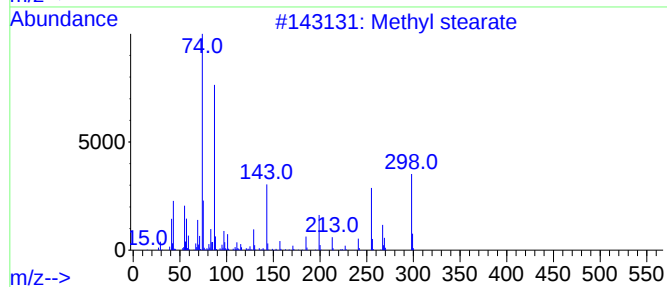
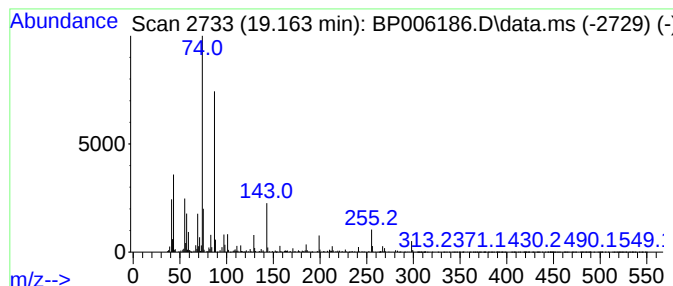
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.163	2.49 ng	251330	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006186.D
Acq On : 12 Jul 2021 17:56
Operator : CG/JU
Sample : M3002-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-F

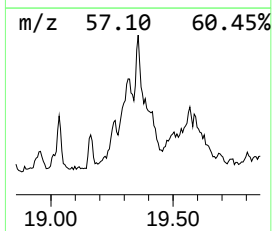
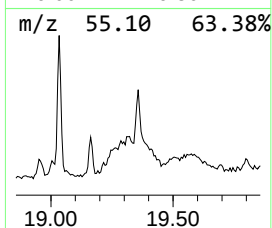
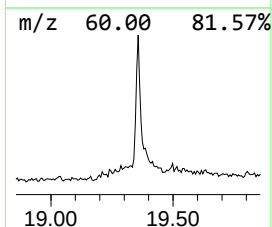
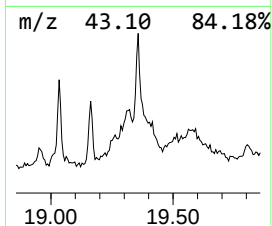
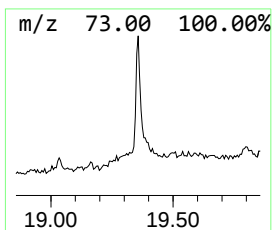
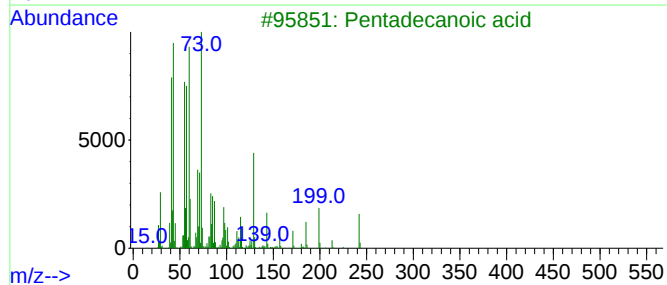
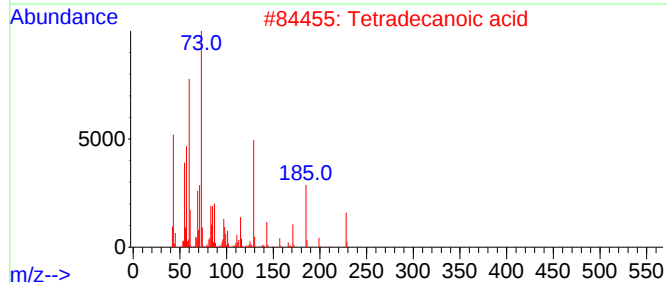
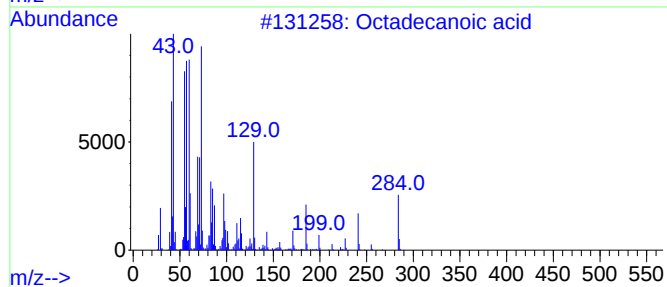
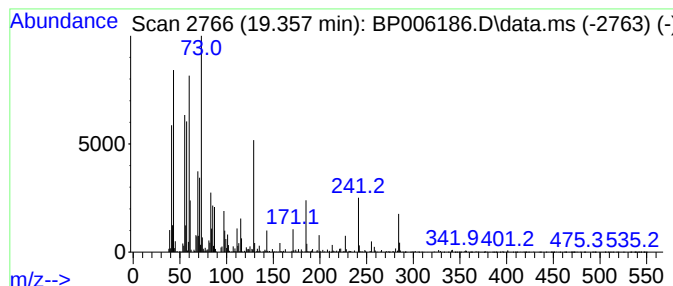
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	3.76 ng	389758	Chrysene-d12	21.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
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Operator : CG/JU
Sample : M3002-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-F

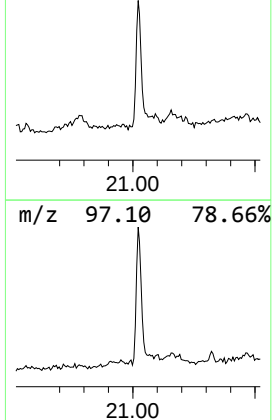
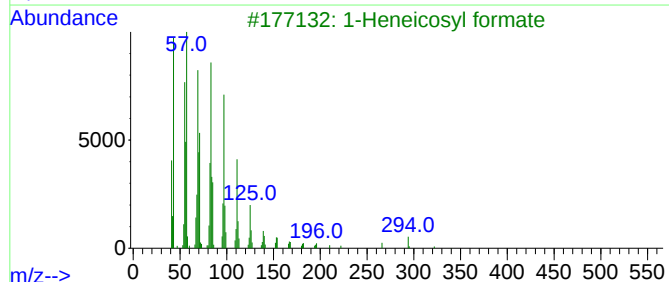
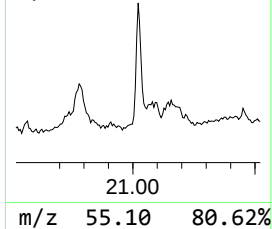
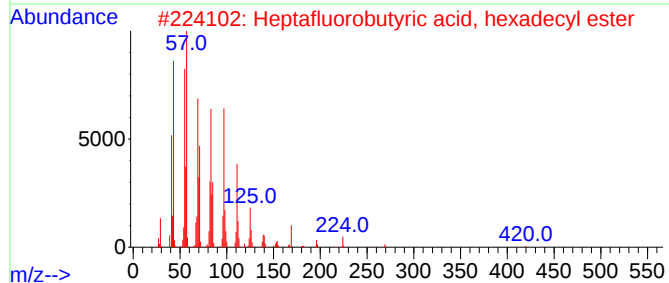
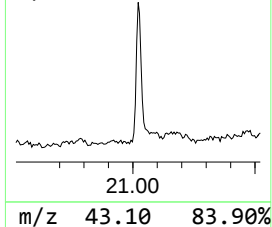
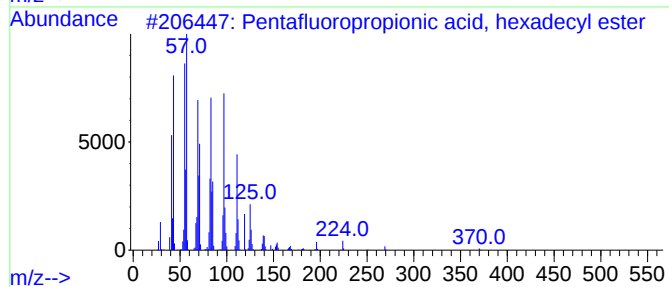
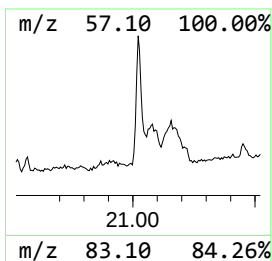
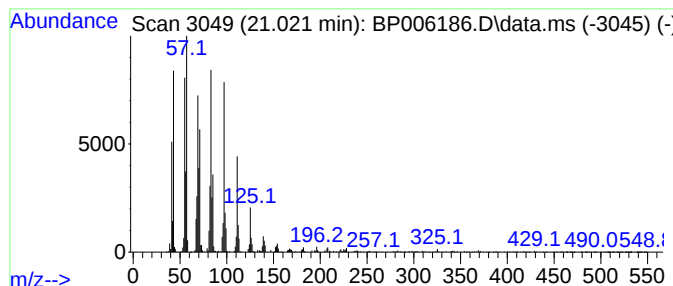
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	8.57 ng	888763	Chrysene-d12	21.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
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Sample : M3002-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-F

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
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2,4,7,9-Tetrame...	13.398	6.7	ng	620614	3	14.498	1863400	20.0
Hexadecanoic ac...	17.904	3.5	ng	350509	4	17.245	2015170	20.0
n-Hexadecanoic ...	18.128	11.3	ng	1136130	4	17.245	2015170	20.0
8-Octadecenoic ...	19.033	5.7	ng	578078	4	17.245	2015170	20.0
Methyl stearate	19.163	2.5	ng	251330	4	17.245	2015170	20.0
Octadecanoic acid	19.357	3.8	ng	389758	5	21.322	2073900	20.0
Pentafluoroprop...	21.022	8.6	ng	888763	5	21.322	2073900	20.0