LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
Data File : BP008081.D
Acq On : 22 Nov 2021 14:09
Operator : CG/JU
Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	20	rVB	967929	1210429	19.42%	3.291%
2	5.411	406	412	424	rBV	2150517	3154919	50.63%	8.577%
3	6.999	674	682	697	rBV	1953116	3270039	52.48%	8.890%
4	7.822	814	822	830	rBV	476633	745012	11.96%	2.025%
5	8.981	1010	1019	1029	rBV	1230337	2055583	32.99%	5.588%
6	10.410	1255	1262	1272	rBV2	31686	72100	1.16%	0.196%
7	10.616	1290	1297	1307	rBV	589704	965354	15.49%	2.624%
8	13.087	1709	1717	1728	rBV	2731402	4104091	65.86%	11.157%
9	14.463	1944	1951	1958	rBV	840066	1221304	19.60%	3.320%
10	15.287	2083	2091	2095	rBV2	46779	94418	1.52%	0.257%
11	15.957	2198	2205	2225	rBV	2157868	3225040	51.75%	8.767%
12	17.222	2414	2420	2430	rBV	1018732	1496868	24.02%	4.069%
13	17.345	2437	2441	2448	rVB4	47624	76458	1.23%	0.208%
14	18.116	2568	2572	2579	rBV	181580	267381	4.29%	0.727%
15	18.186	2580	2584	2589	rVB	49348	65290	1.05%	0.177%
16	19.239	2759	2763	2771	rBV2	42065	72200	1.16%	0.196%
17	19.351	2779	2782	2789	rBV2	85051	127869	2.05%	0.348%
18	19.786	2851	2856	2868	rBV	4902168	6231471	100.00%	16.940%
19	20.469	2968	2972	2977	rBV	155765	196146	3.15%	0.533%
20	20.539	2981	2984	2987	rVV	82305	95126	1.53%	0.259%
21	20.580	2988	2991	2996	rVB	126487	136118	2.18%	0.370%
22	21.033	3064	3068	3075	rBV2	578606	796114	12.78%	2.164%
23	21.098	3075	3079	3085	rVB	239093	313773	5.04%	0.853%
24	21.233	3099	3102	3106	rBV	178767	191217	3.07%	0.520%
25	21.316	3110	3116	3120	rBV	1618295	2226770	35.73%	6.054%
26	21.351	3120	3122	3130	rVB	208242	278323	4.47%	0.757%
27	21.475	3139	3143	3148	rVB	261432	296575	4.76%	0.806%
28	21.933	3218	3221	3231	rBV	208803	316566	5.08%	0.861%
29	22.157	3256	3259	3267	rVB	184973	249852	4.01%	0.679%
30	22.427	3301	3305	3313	rVB2	535998	825890	13.25%	2.245%
31	22.986	3396	3400	3405	rBV2	228709	398019	6.39%	1.082%
32	23.716	3517	3524	3533	rVB2	966779	2008413	32.23%	5.460%

Sum of corrected areas: 36784728

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
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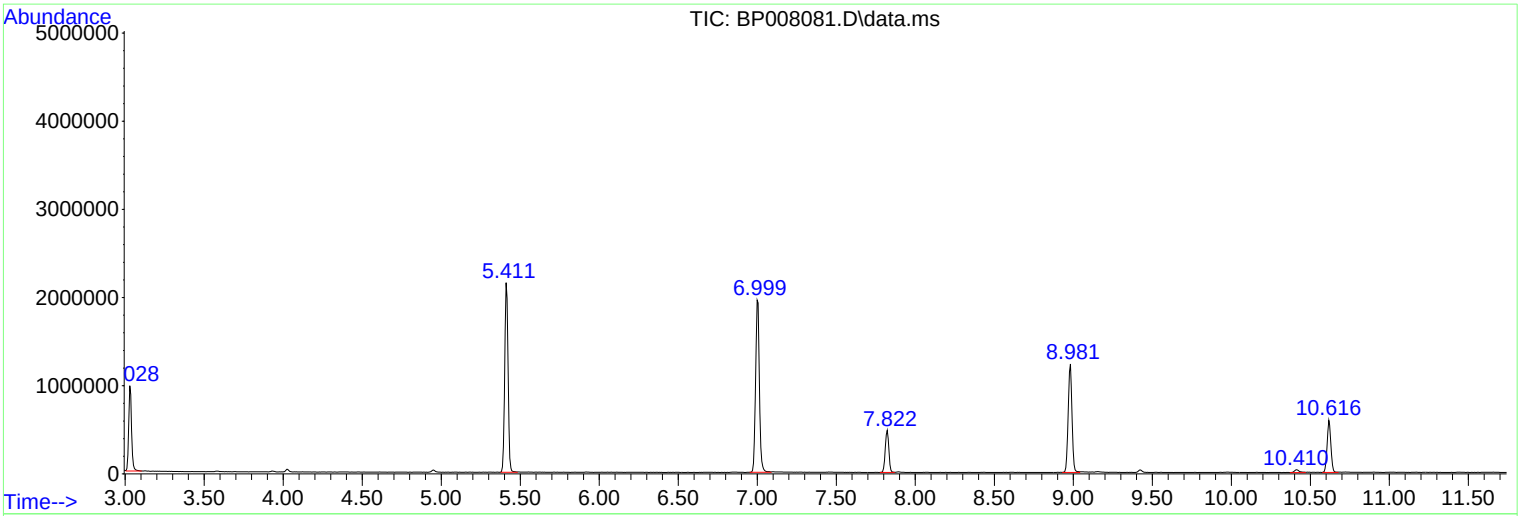
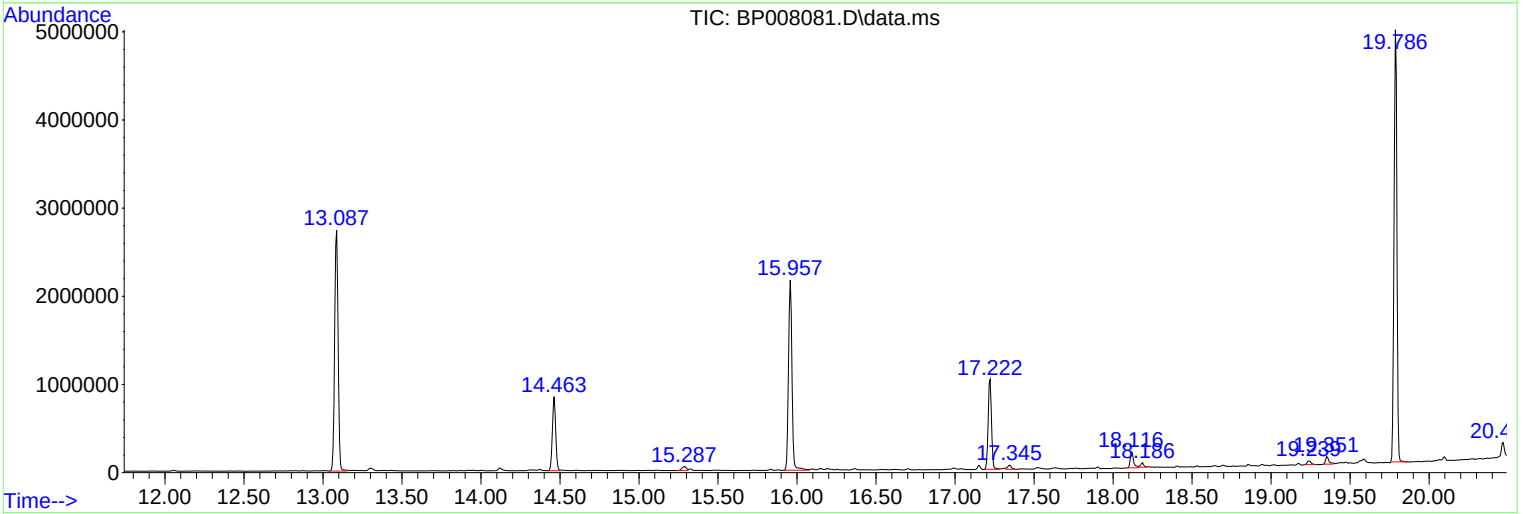
Operator : CG/JU
Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

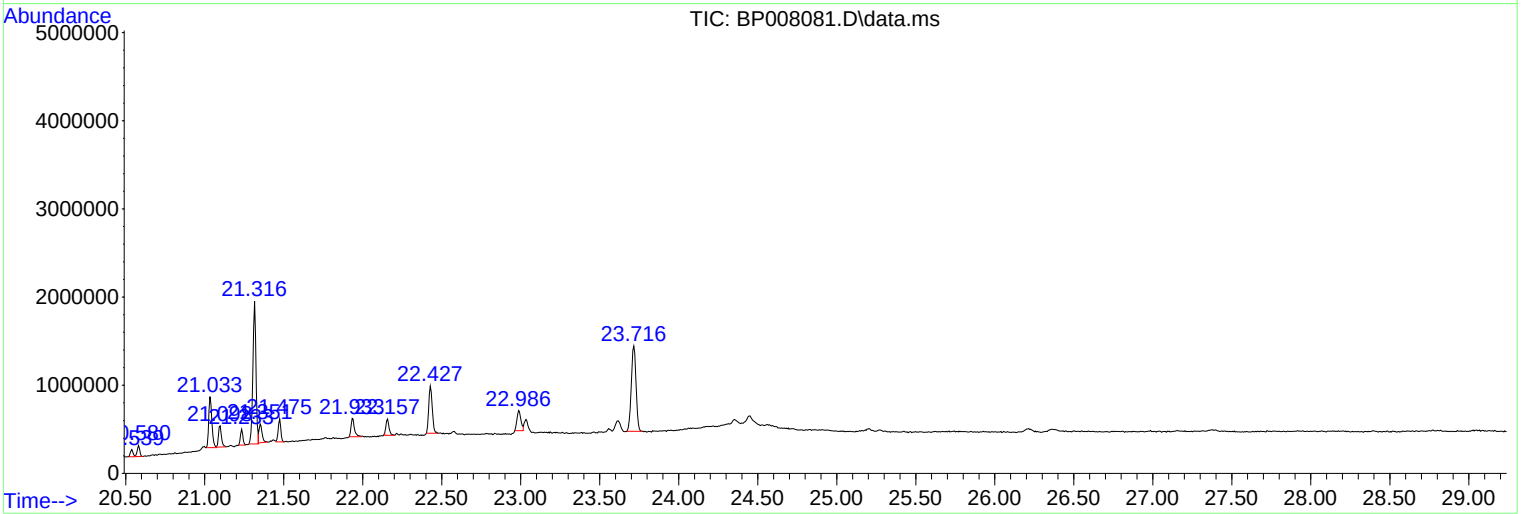
Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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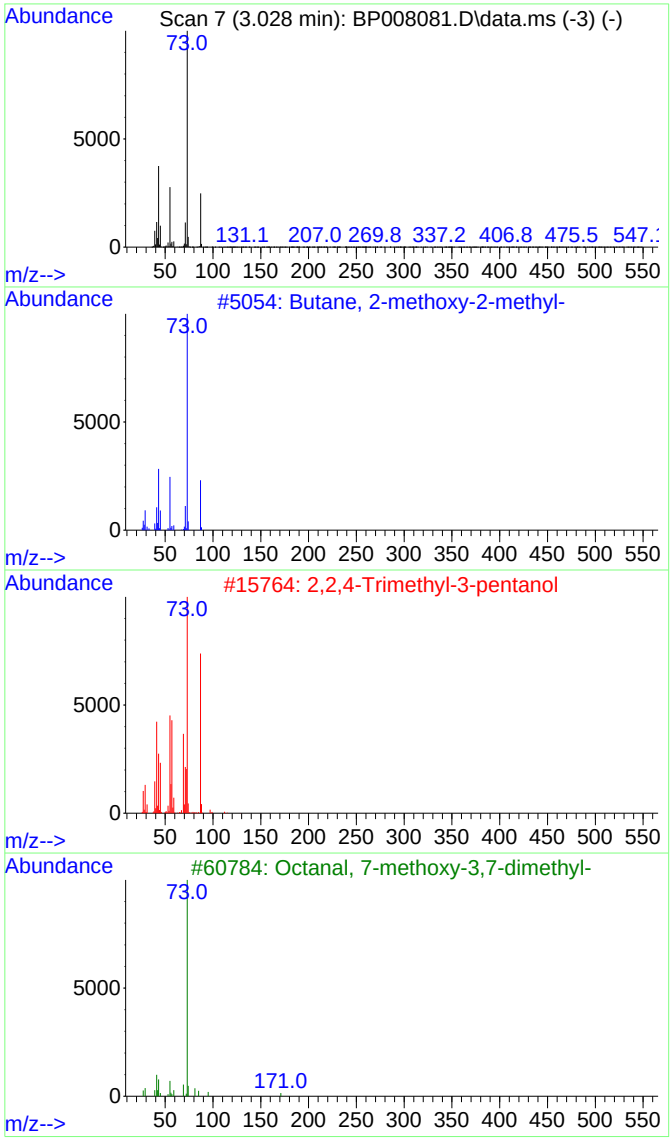
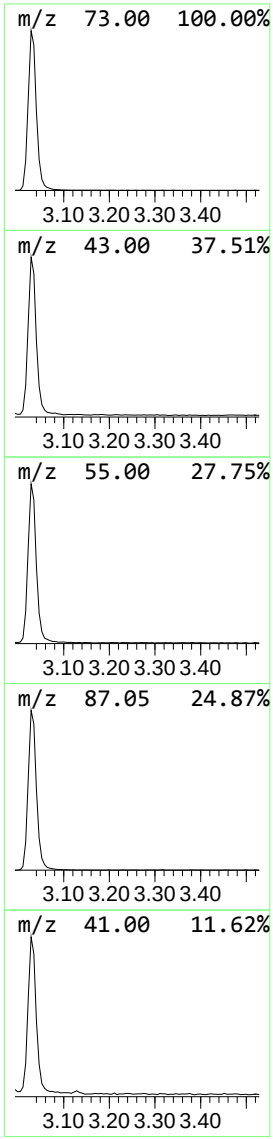
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	32.49 ng	1210430	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BP008081.D
Acq On : 22 Nov 2021 14:09
Operator : CG/JU
Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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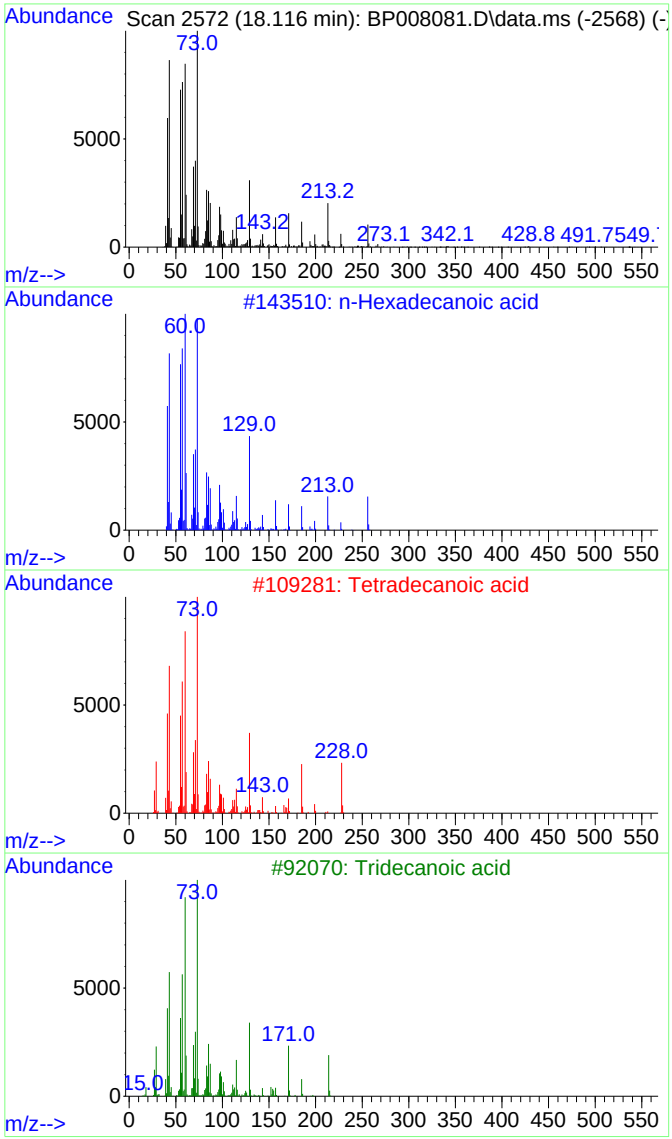
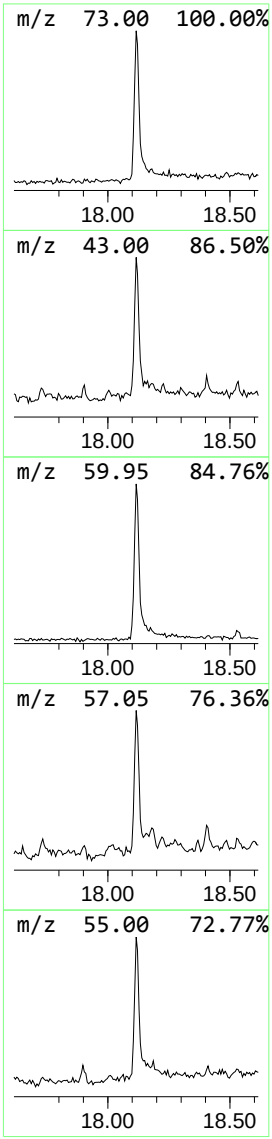
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	3.57 ng	267381	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83





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Sample : M4754-02
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Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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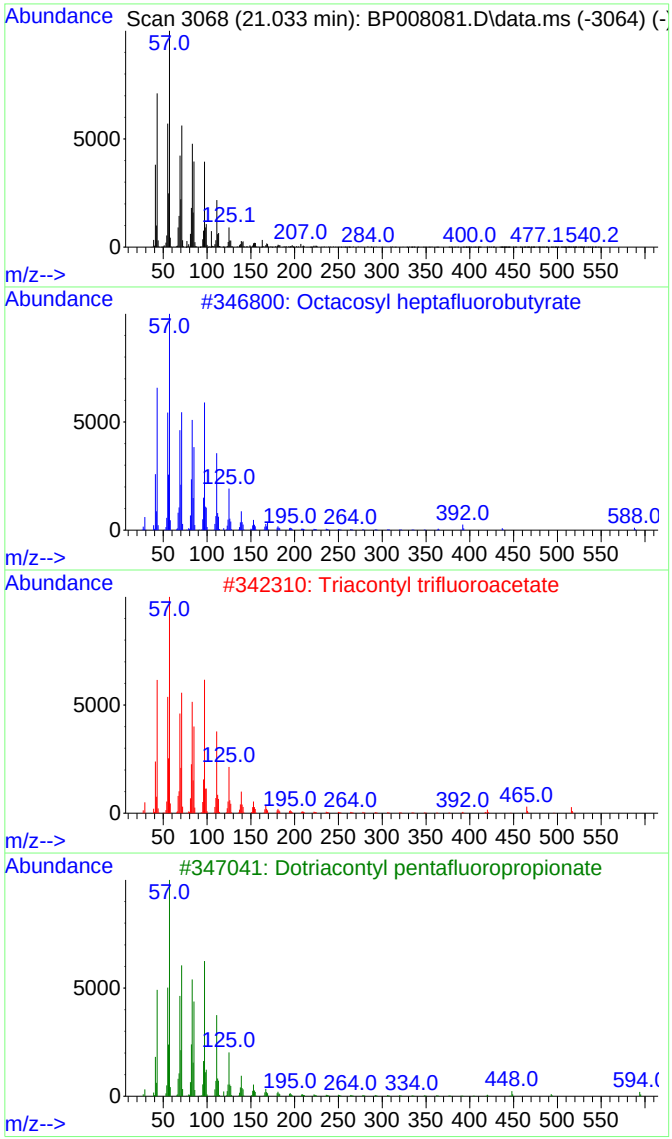
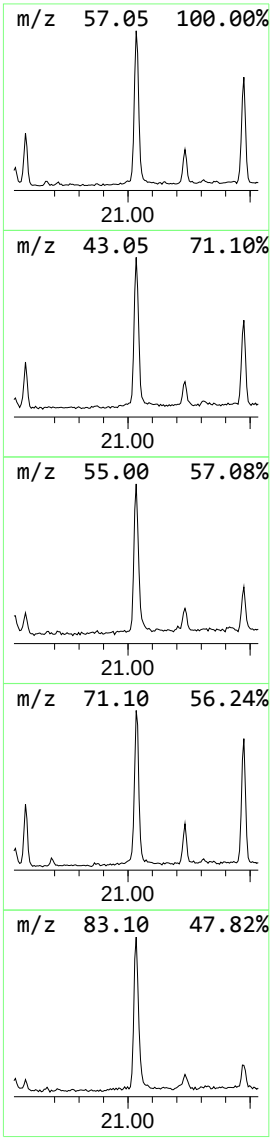
Peak Number 3 Octacosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	7.15 ng	796114	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
2	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
Data File : BP008081.D
Acq On : 22 Nov 2021 14:09
Operator : CG/JU
Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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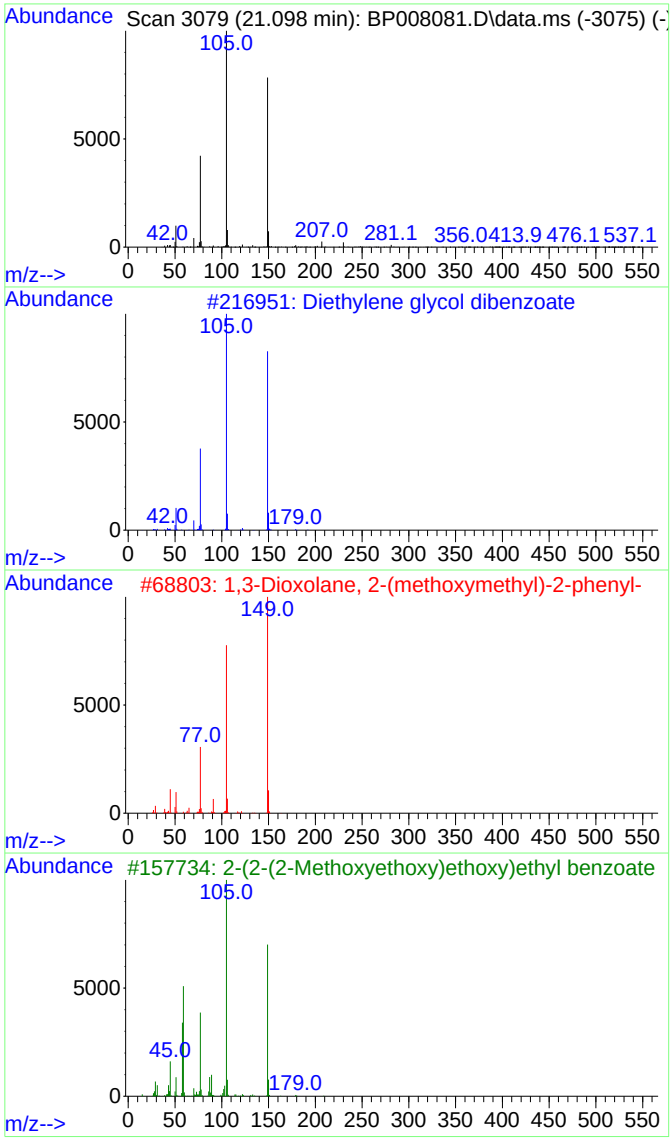
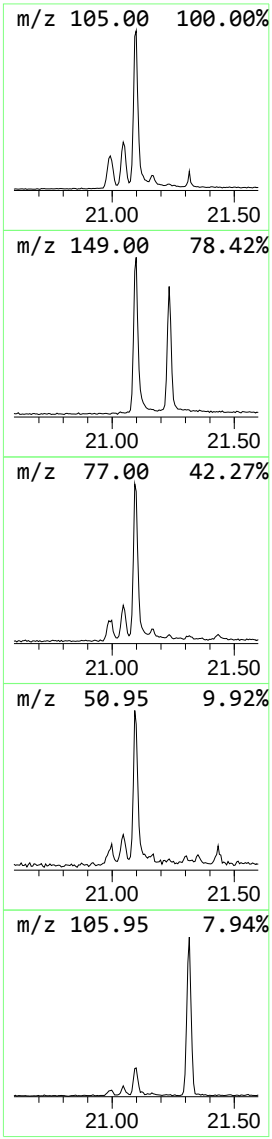
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	2.82 ng	313773	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	74
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
5	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	64





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Data File : BP008081.D
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Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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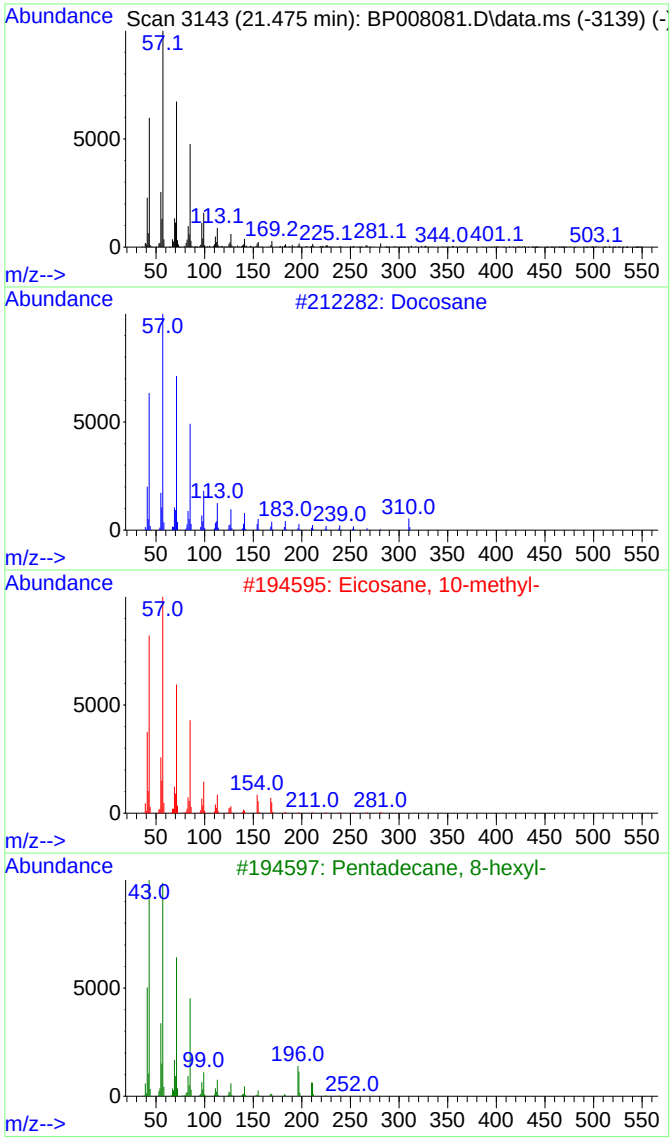
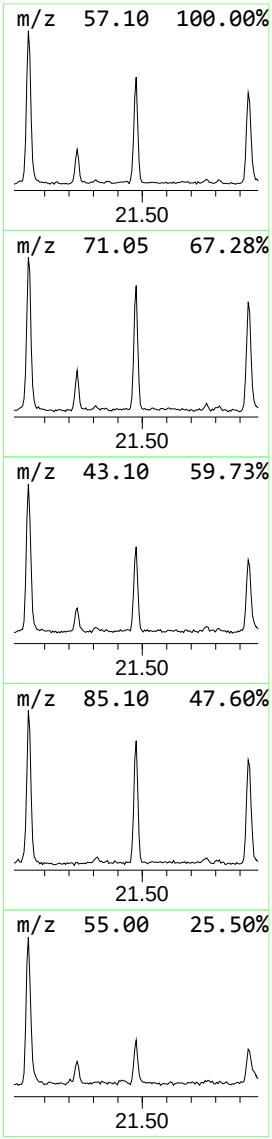
Peak Number 5 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	2.66 ng	296575	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
4	9-Methylheneicosane	310	C22H46	070475-51-3	90
5	Octacosane	394	C28H58	000630-02-4	90





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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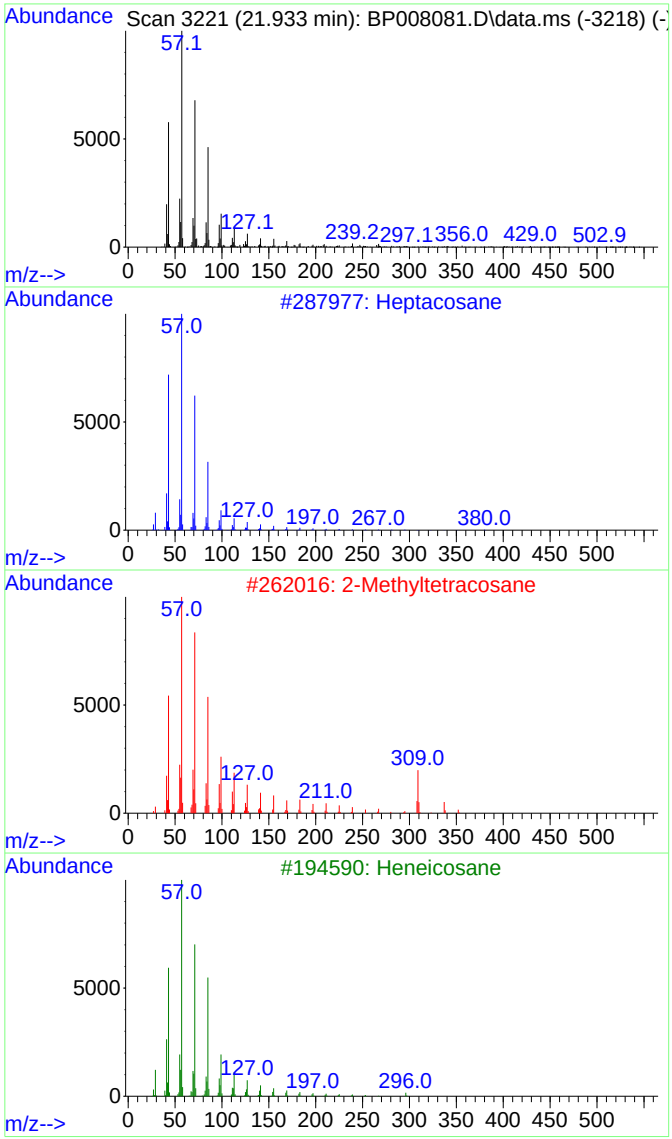
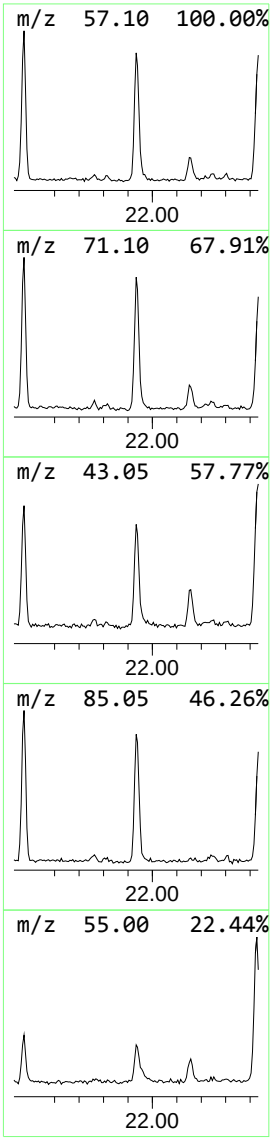
Peak Number 6 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.933	2.84 ng	316566	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	95
2	2-Methyltetracosane	352	C25H52	001560-78-7	93
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : M4754-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-12-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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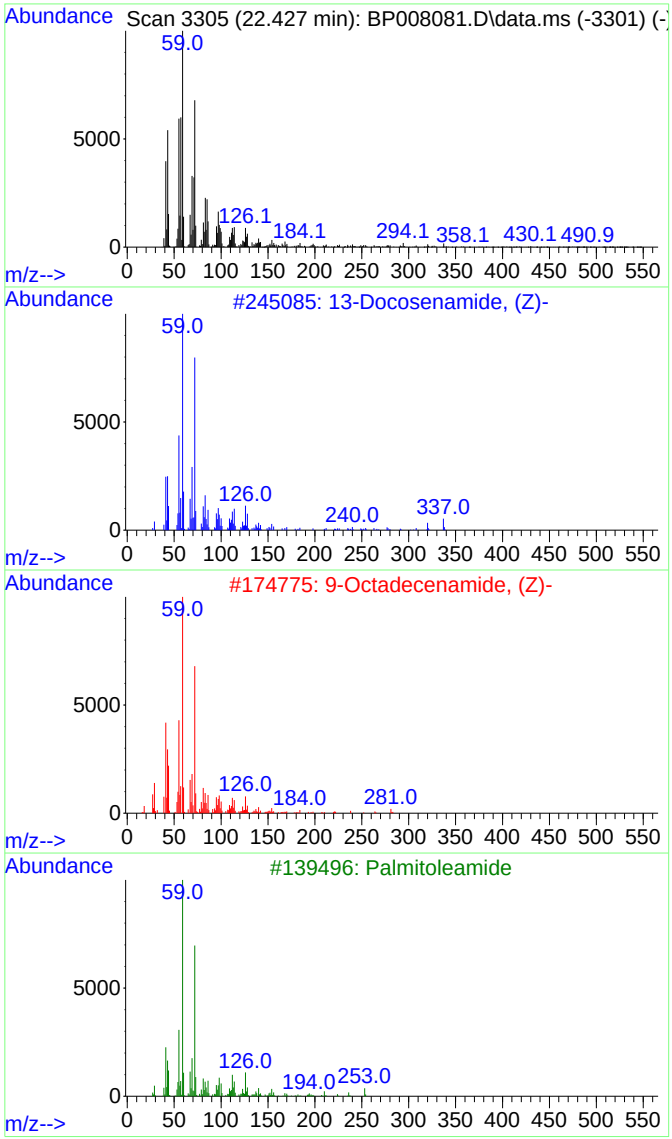
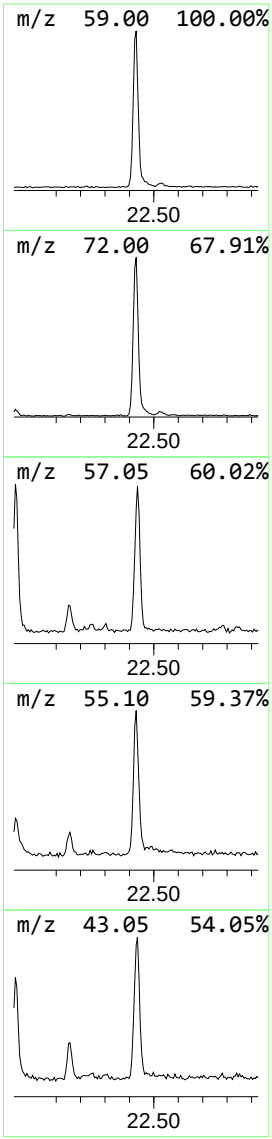
Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	7.42 ng	825890	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3	Palmitoleamide	253	C16H31NO	106010-22-4	52
4	Dodecanamide	199	C12H25NO	001120-16-7	47
5	Nonanamide	157	C9H19NO	001120-07-6	43





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.028	32.5	ng	1210430	1	7.822	745012	20.0
n-Hexadecanoic ...	18.116	3.6	ng	267381	4	17.222	1496870	20.0
Octacosyl hepta...	21.033	7.2	ng	796114	5	21.316	2226770	20.0
Diethylene glyc...	21.098	2.8	ng	313773	5	21.316	2226770	20.0
Docosane	21.474	2.7	ng	296575	5	21.316	2226770	20.0
Heptacosane	21.933	2.8	ng	316566	5	21.316	2226770	20.0
13-Docosenamide...	22.427	7.4	ng	825890	5	21.316	2226770	20.0