LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008066.D
Acq On : 20 Nov 2021 19:57
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : JC-02-111621

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: BP008066.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.411	355	361	383	rBV	2286890	3367805	47.10%	7.124%
2	6.999	622	631	647	rBV	2145465	3576295	50.02%	7.565%
3	7.822	764	771	779	rBV	493292	779131	10.90%	1.648%
4	8.981	959	968	977	rBV	1354894	2256935	31.56%	4.774%
5	10.405	1204	1210	1229	rBV	574867	981232	13.72%	2.076%
6	10.616	1239	1246	1253	rBV	618357	1041826	14.57%	2.204%
7	13.087	1658	1666	1679	rBV	3052906	4671526	65.33%	9.882%
8	14.463	1892	1900	1906	rBV	883585	1389280	19.43%	2.939%
9	14.781	1948	1954	1960	rBV	74121	110788	1.55%	0.234%
10	15.951	2147	2153	2175	rVB	2432442	3795753	53.09%	8.029%
11	16.522	2245	2250	2255	rBV2	91837	125666	1.76%	0.266%
12	17.216	2362	2368	2373	rBV	1233022	1765358	24.69%	3.734%
13	17.257	2373	2375	2381	rVV	134842	167031	2.34%	0.353%
14	17.345	2385	2390	2396	rVB3	82627	133737	1.87%	0.283%
15	17.898	2480	2484	2489	rBV	150428	178678	2.50%	0.378%
16	18.116	2513	2521	2529	rBV2	222153	365801	5.12%	0.774%
17	19.028	2673	2676	2681	rVB	158238	186460	2.61%	0.394%
18	19.228	2705	2710	2718	rBV	272315	386344	5.40%	0.817%
19	19.351	2727	2731	2734	rBV	72646	86435	1.21%	0.183%
20	19.580	2763	2770	2779	rVB	238063	359632	5.03%	0.761%
21	19.780	2799	2804	2817	rVB	5565759	7150248	100.00%	15.125%
22	21.027	3012	3016	3023	rVV2	487845	695328	9.72%	1.471%
23	21.086	3023	3026	3034	rVB	203786	278724	3.90%	0.590%
24	21.310	3058	3064	3068	rBV	1609529	2184879	30.56%	4.622%
25	21.469	3087	3091	3097	rVB	207819	257473	3.60%	0.545%
26	21.927	3165	3169	3181	rVB	337661	491509	6.87%	1.040%
27	22.427	3250	3254	3260	rVB	499825	649232	9.08%	1.373%
28	22.980	3343	3348	3360	rVB2	737242	1455086	20.35%	3.078%
29	23.610	3449	3455	3463	rVB2	727957	1430964	20.01%	3.027%
30	23.704	3464	3471	3480	rVB2	968850	1941521	27.15%	4.107%
31	24.339	3573	3579	3587	rVB	729557	1530443	21.40%	3.237%
32	25.186	3717	3723	3733	rVB	668466	1610703	22.53%	3.407%
33	26.180	3885	3892	3906	rVB2	623506	1872496	26.19%	3.961%

Sum of corrected areas: 47274319

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
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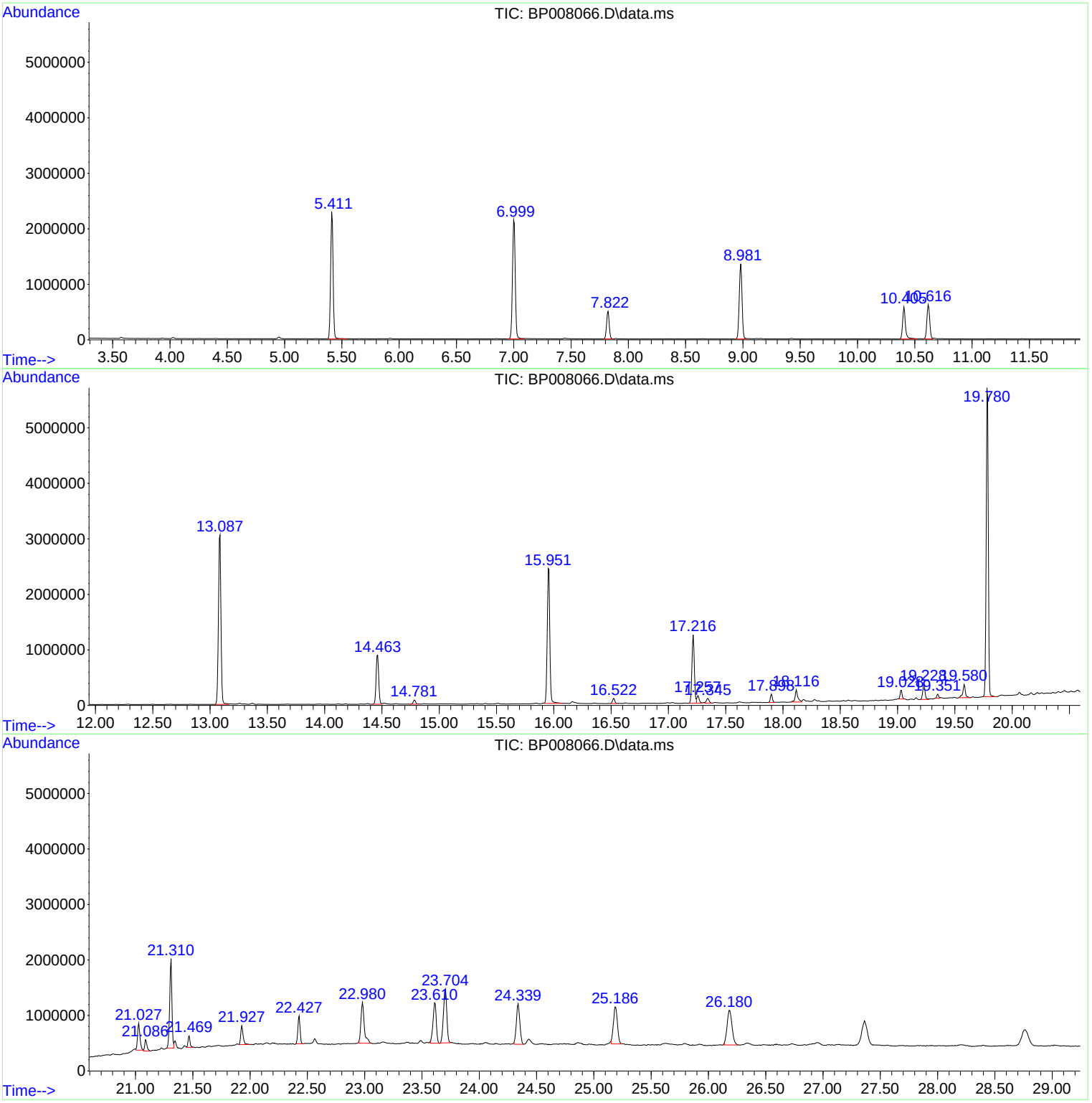
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

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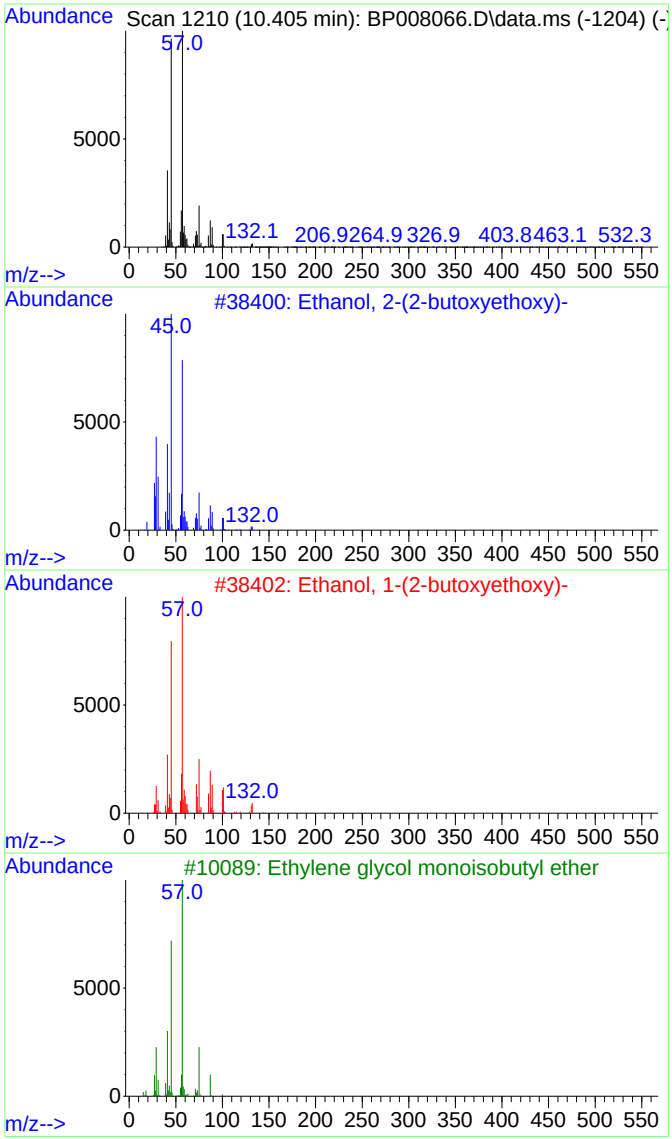
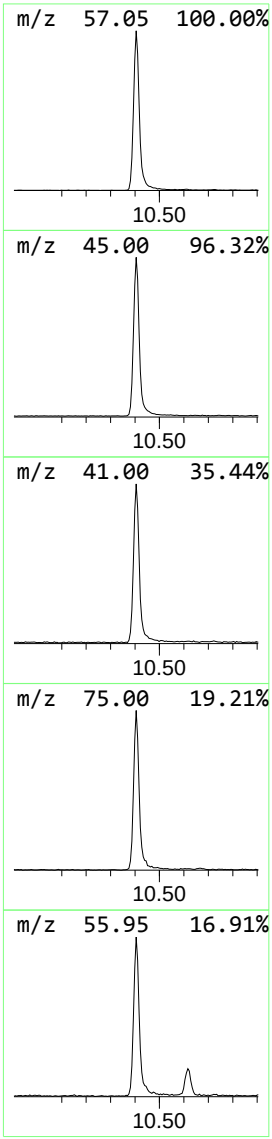
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.405	18.84 ng	981232	Naphthalene-d8	10.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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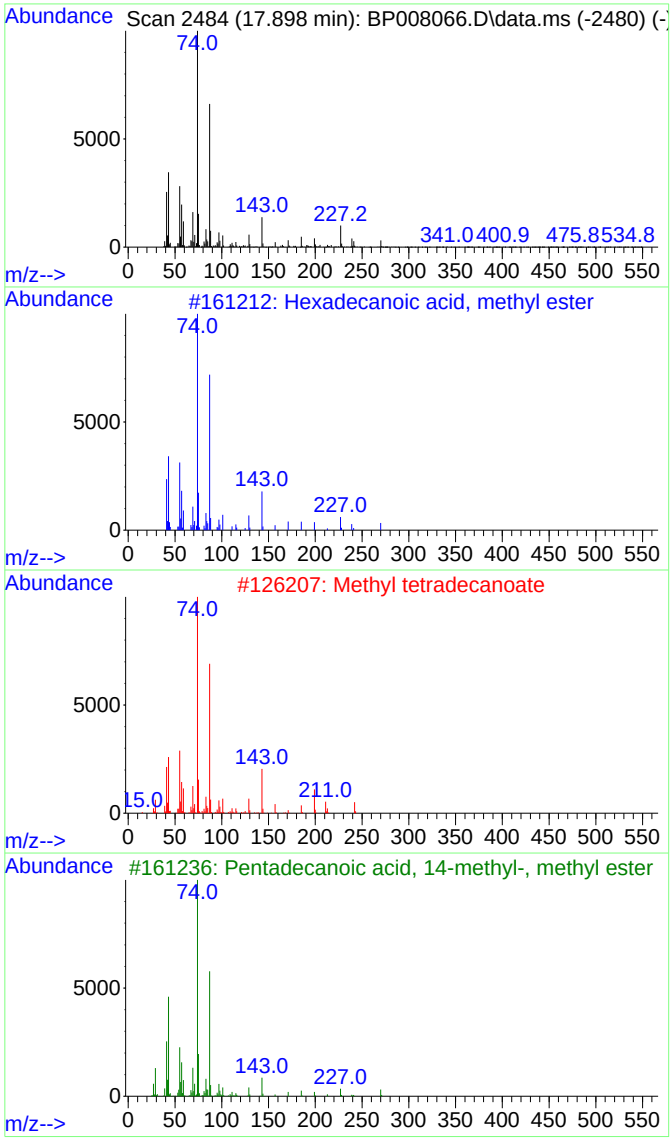
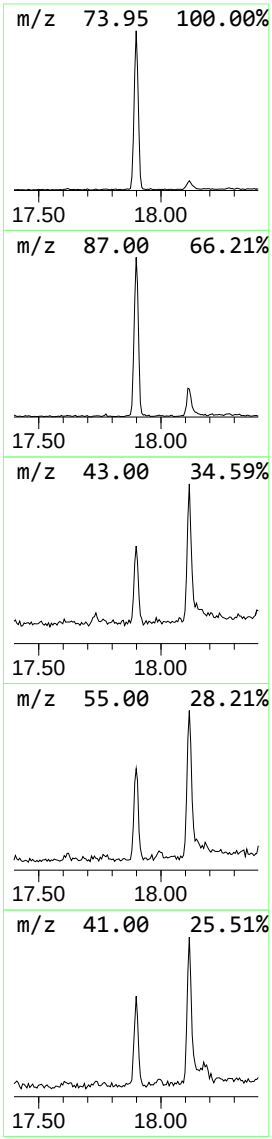
****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.898	2.02 ng	178678	Phenanthrene-d10	17.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87





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Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Integration Parameters: LSCINT.P

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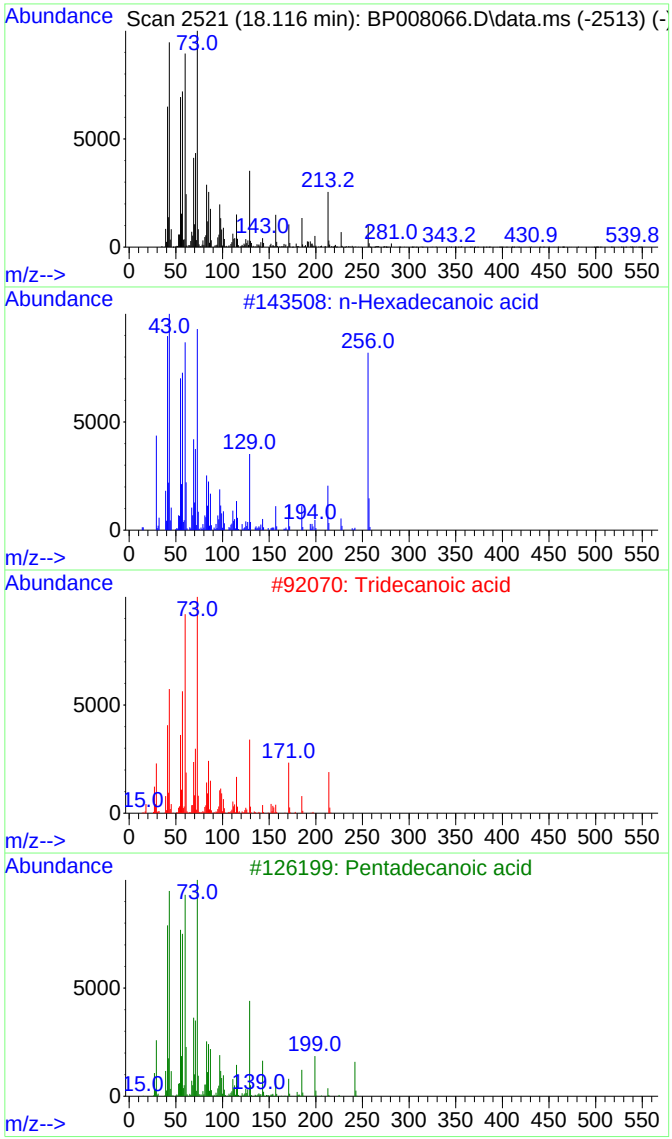
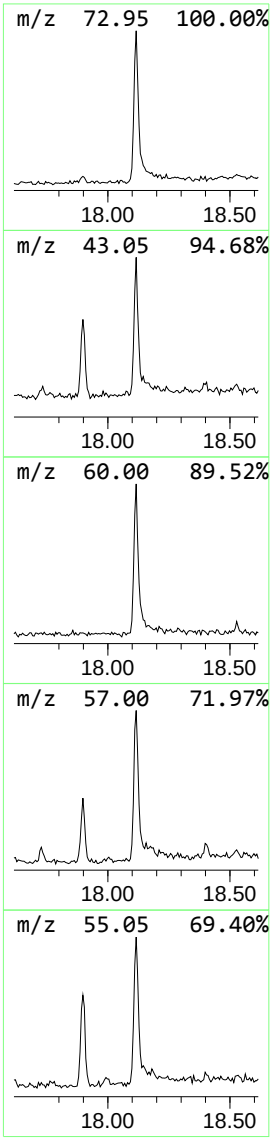
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	4.14 ng	365801	Phenanthrene-d10	17.216

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	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	59





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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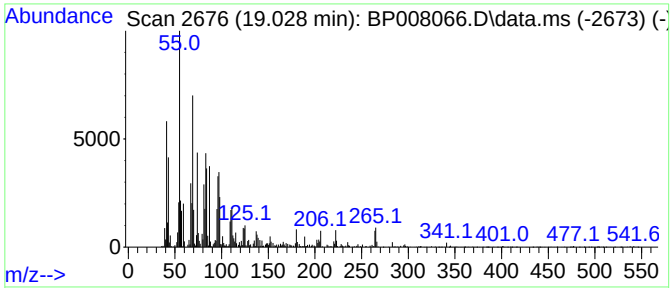
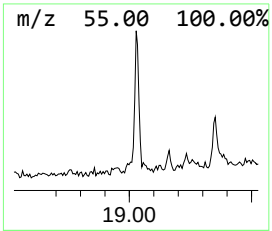
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

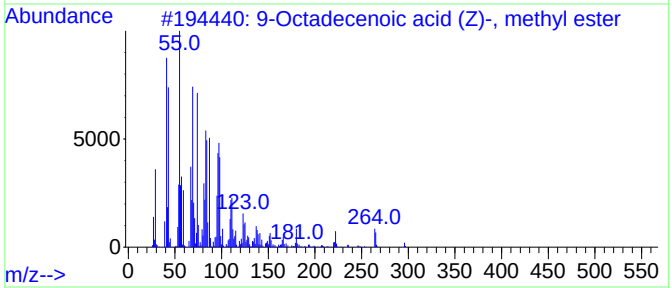
****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 11

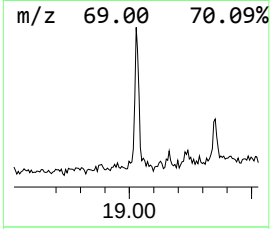
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.028	2.11 ng	186460	Phenanthrene-d10	17.216

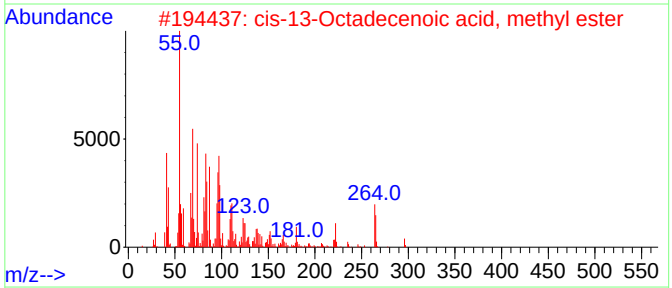
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
4	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	98
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98

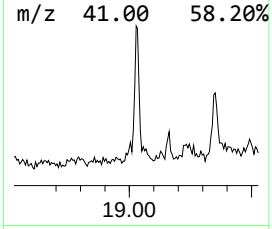


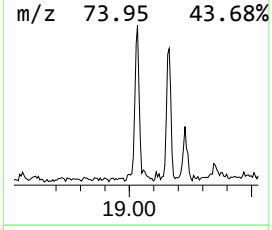


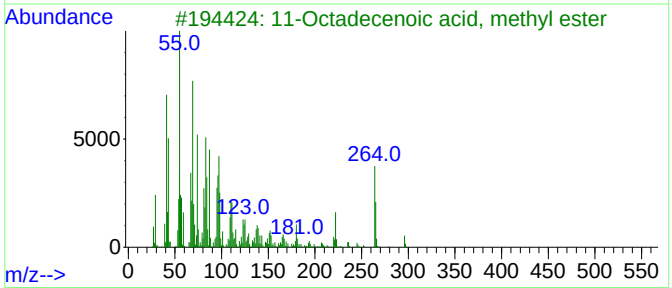


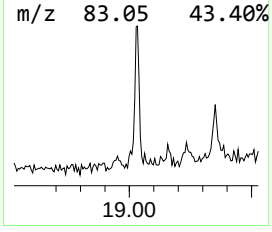












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

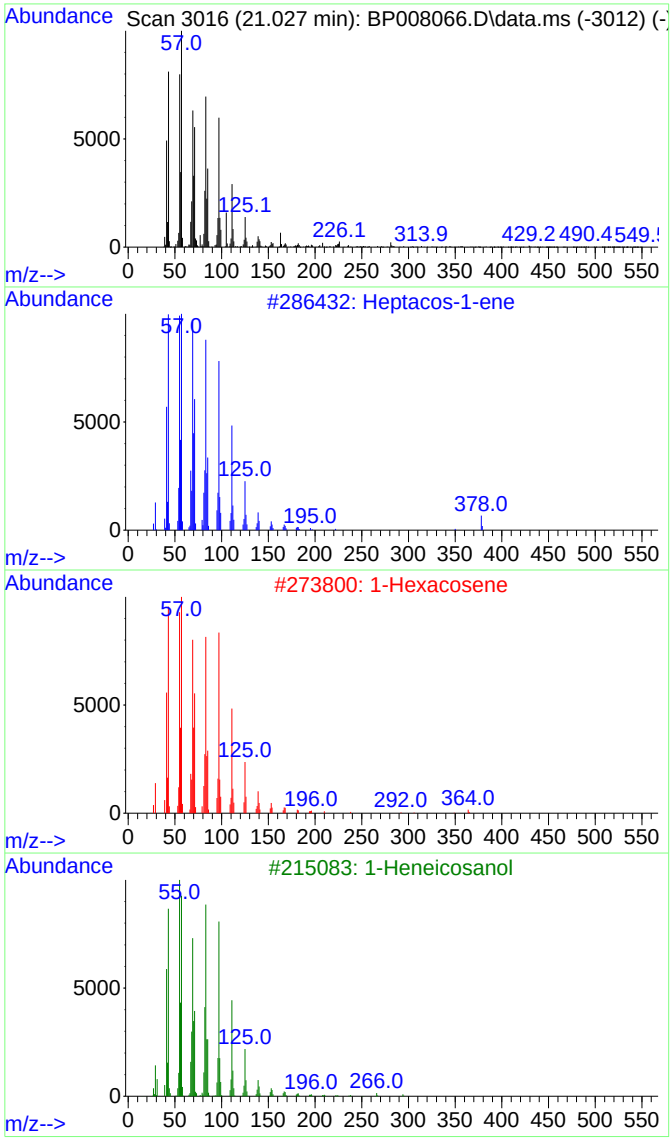
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

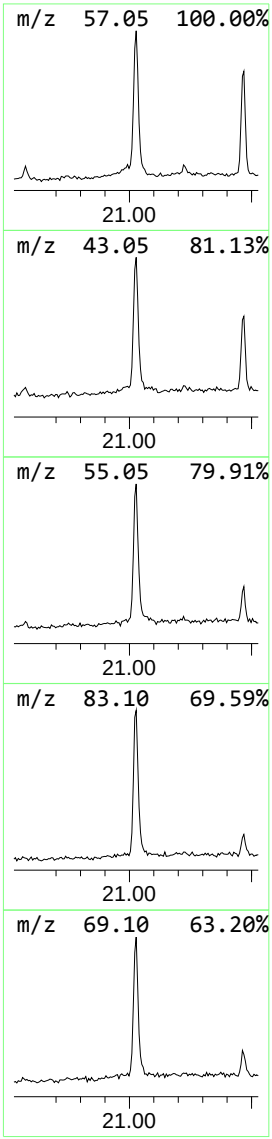
****

Peak Number 5 Heptacos-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.028	6.36 ng	695328	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





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

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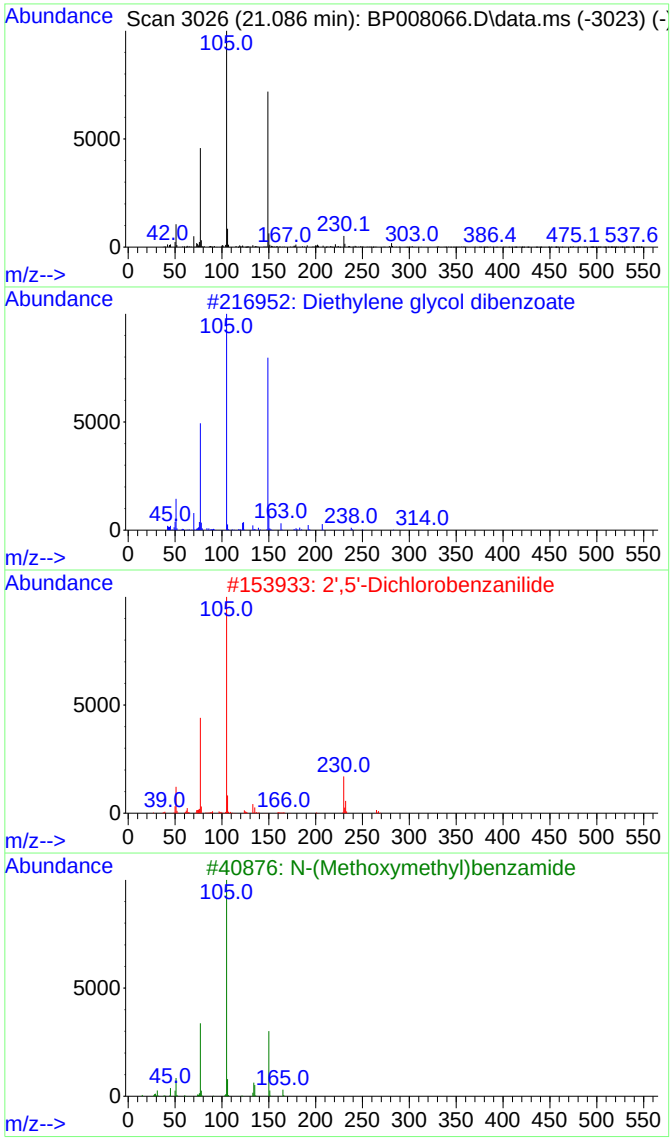
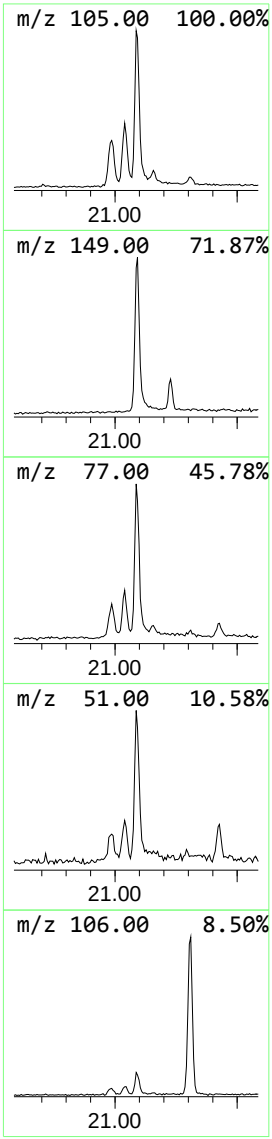
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	2.55 ng	278724	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	2',5'-Dichlorobenzanilide	265	C13H9Cl2NO	006626-75-1	47
3	N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	47
4	N'-Benzoyl-2-furohydrazide	230	C12H10N2O3	113643-84-8	47
5	1,3-propanedione, 2-(acetyloxy)-...	282	C17H14O4	1000401-92-5	46





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TIC Library : C:\Database\NIST20.L
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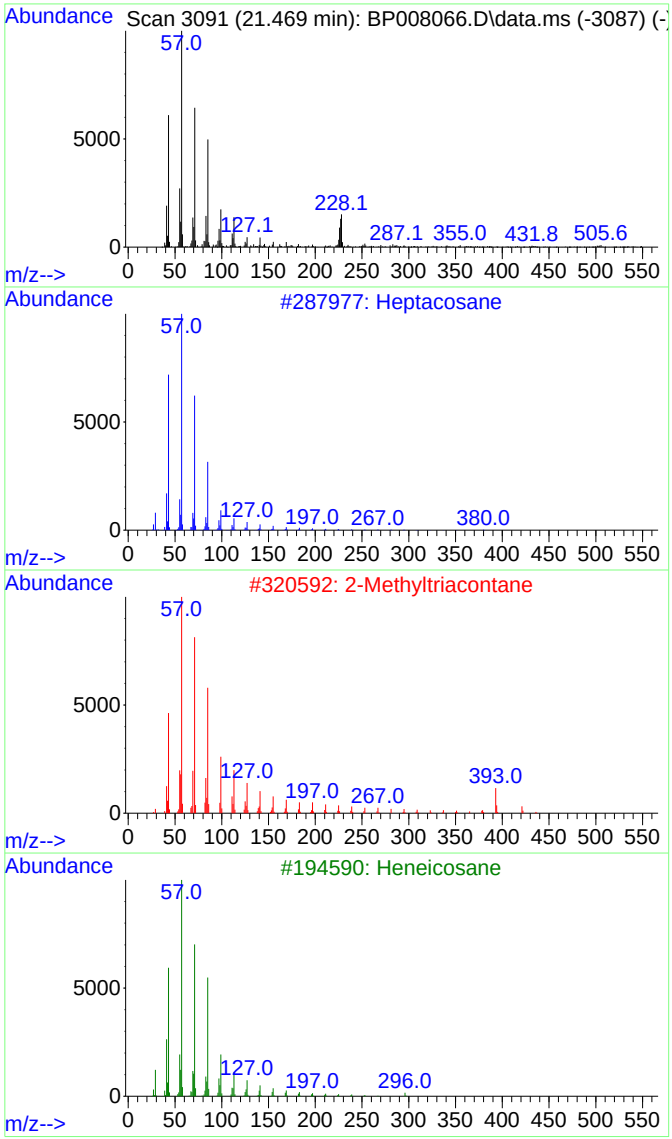
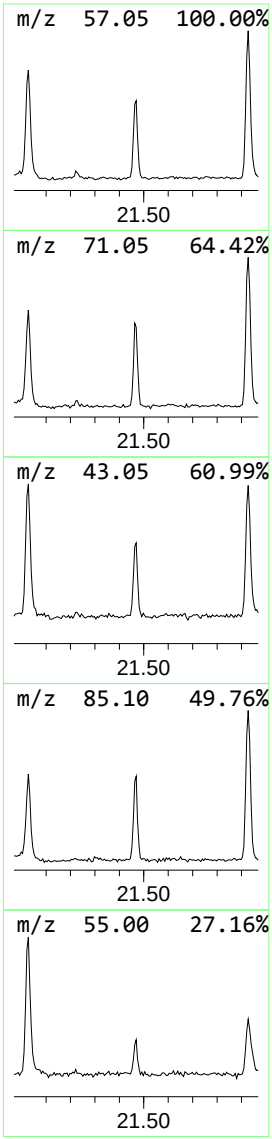
Peak Number 7 2-Methyltriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.469	2.36 ng	257473	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	2-Methyltriacontane	437	C31H64	001560-72-1	74
3	Heneicosane	296	C21H44	000629-94-7	74
4	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	74
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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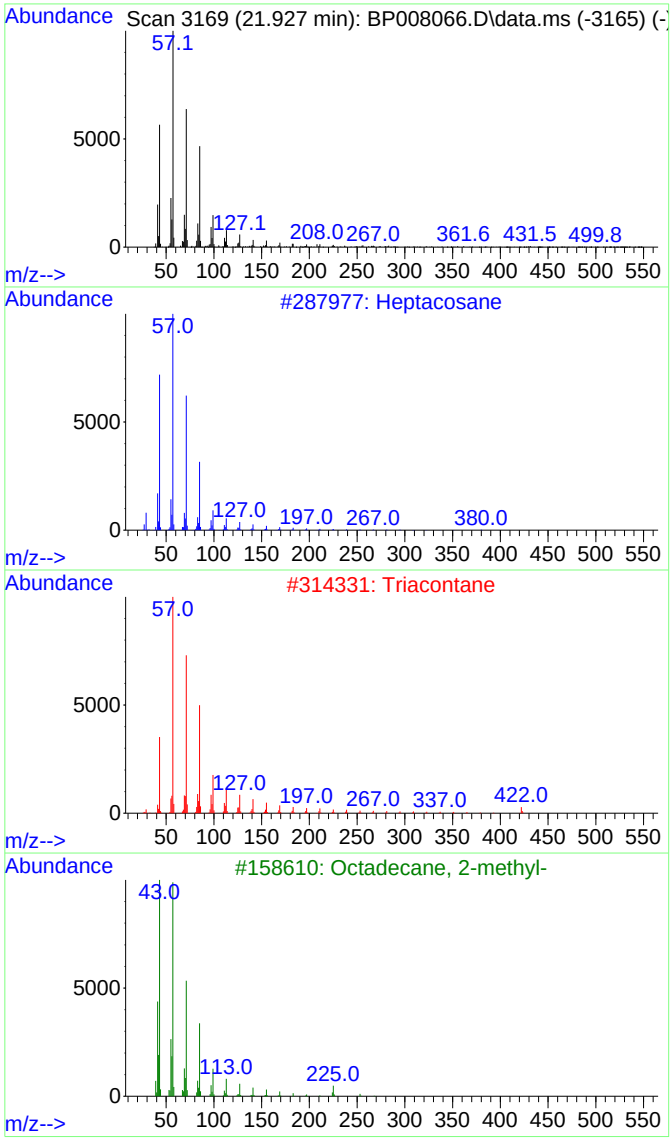
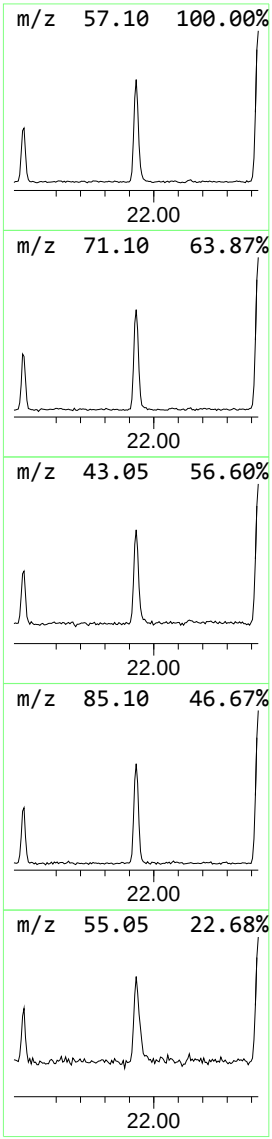
Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.927	4.50 ng	491509	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	98
2	Triacontane	422	C30H62	000638-68-6	96
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
5	Nonacosane	408	C29H60	000630-03-5	91





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Data File : BP008066.D
Acq On : 20 Nov 2021 19:57
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

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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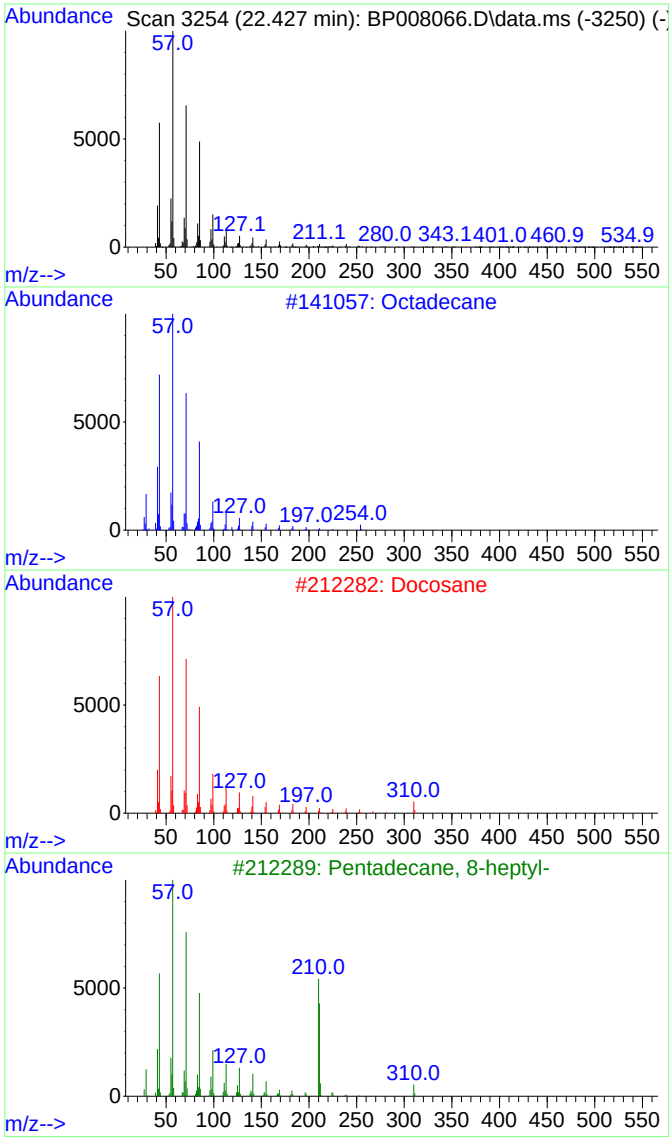
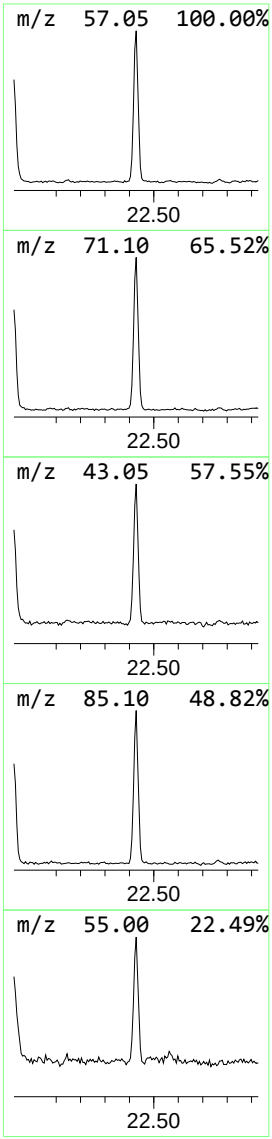
Peak Number 9 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	5.94 ng	649232	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	97
2	Docosane	310	C22H46	000629-97-0	95
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	94
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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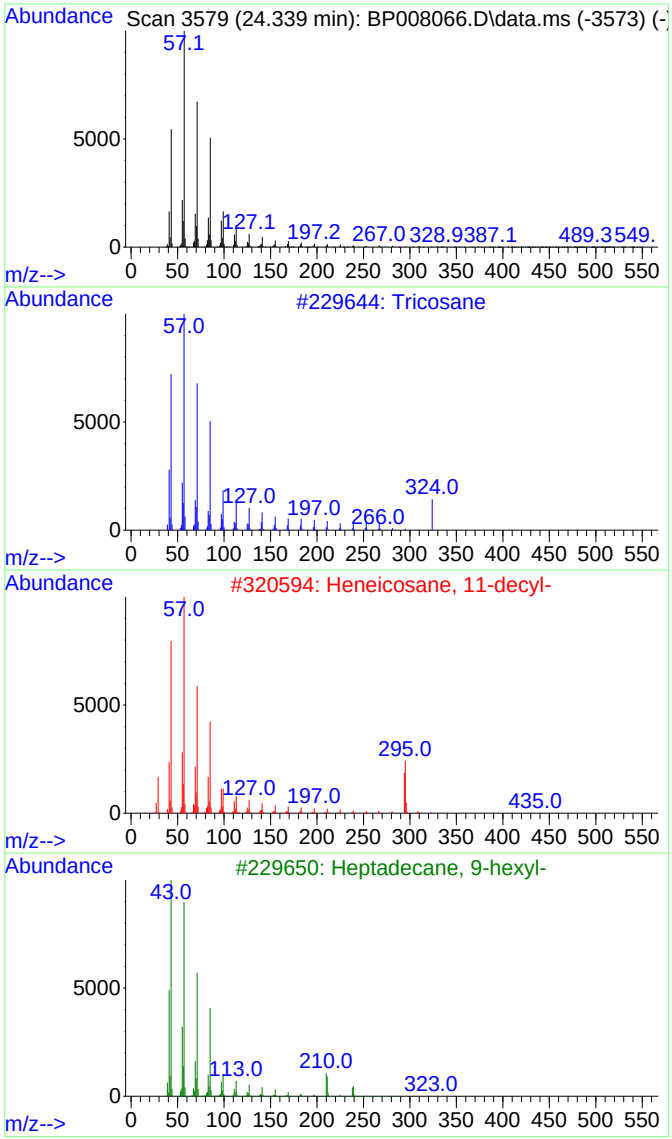
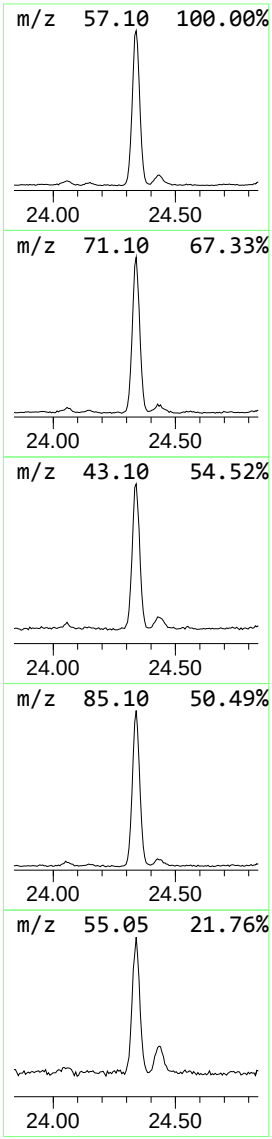
Peak Number 10 Heneicosane, 11-decyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.339	15.77 ng	1530440	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	95
2	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	95
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Octacosane	394	C28H58	000630-02-4	91





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Data File : BP008066.D
Acq On : 20 Nov 2021 19:57
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

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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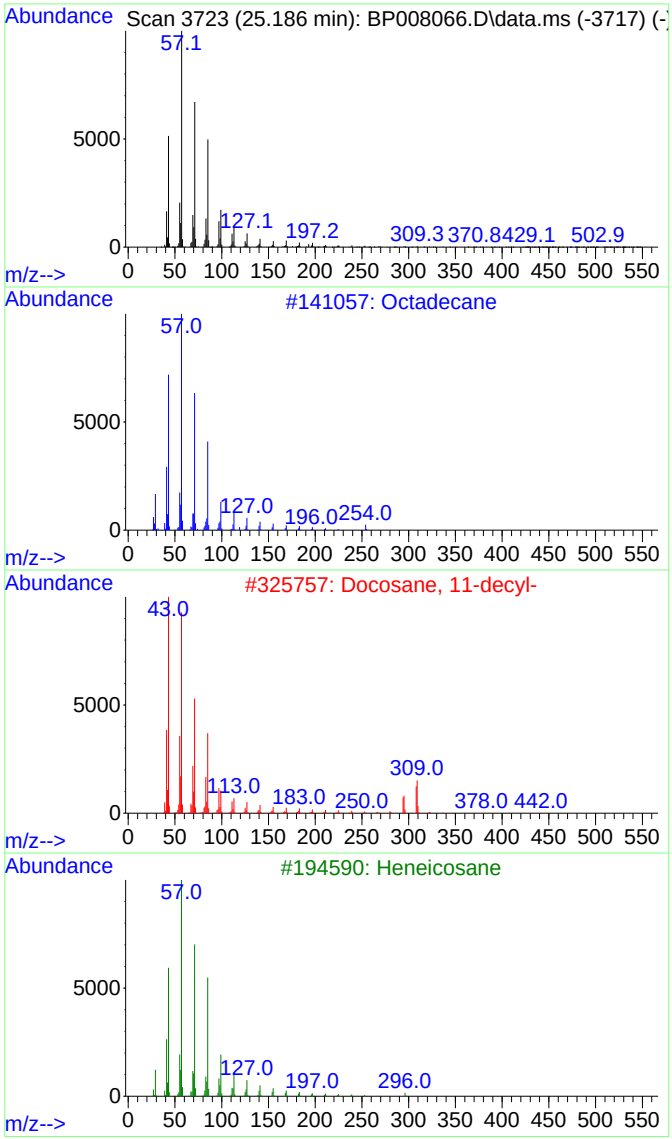
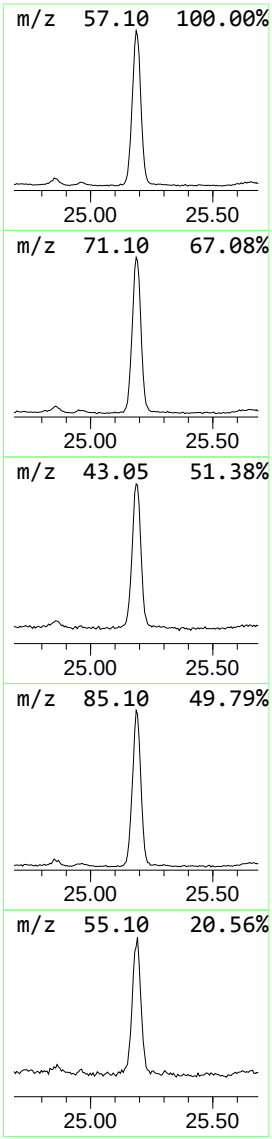
Peak Number 11 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.186	16.59 ng	1610700	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





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Data File : BP008066.D
Acq On : 20 Nov 2021 19:57
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

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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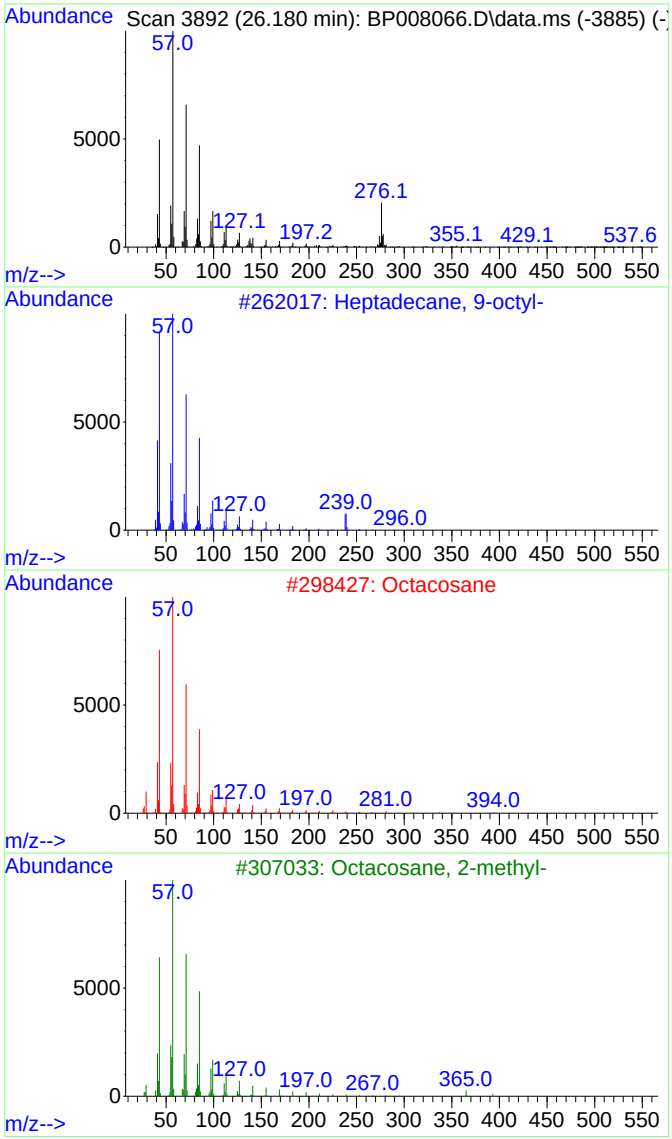
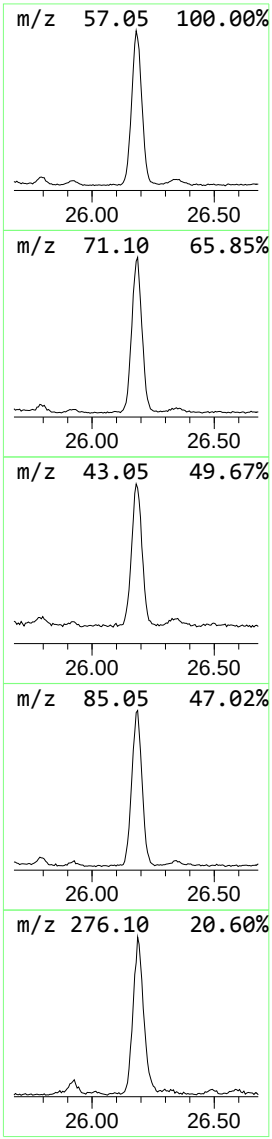
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.180	19.29 ng	1872500	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2	Octacosane	394	C28H58	000630-02-4	76
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	76
4	Tetracosane	338	C24H50	000646-31-1	76
5	Hexacosane	366	C26H54	000630-01-3	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008066.D
Acq On : 20 Nov 2021 19:57
Operator : CG/JU
Sample : M4708-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JC-02-111621

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
Ethanol, 2-(2-b...	10.405	18.8	ng	981232	2	10.616	1041830	20.0
Hexadecanoic ac...	17.898	2.0	ng	178678	4	17.216	1765360	20.0
n-Hexadecanoic ...	18.116	4.1	ng	365801	4	17.216	1765360	20.0
9-Octadecenoic ...	19.028	2.1	ng	186460	4	17.216	1765360	20.0
Heptacos-1-ene	21.028	6.4	ng	695328	5	21.310	2184880	20.0
Diethylene glyc...	21.086	2.5	ng	278724	5	21.310	2184880	20.0
2-Methyltriacon...	21.469	2.4	ng	257473	5	21.310	2184880	20.0
Heptacosane	21.927	4.5	ng	491509	5	21.310	2184880	20.0
Docosane	22.427	5.9	ng	649232	5	21.310	2184880	20.0
Heneicosane, 11...	24.339	15.8	ng	1530440	6	23.704	1941520	20.0
Octadecane	25.186	16.6	ng	1610700	6	23.704	1941520	20.0
Heptadecane, 9-...	26.180	19.3	ng	1872500	6	23.704	1941520	20.0