LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.452	361	368	377	rBV	3032345	4326154	23.26%	4.604%
2	7.046	631	639	652	rBV	2719938	4281185	23.02%	4.557%
3	7.863	771	778	786	rVB	476158	744466	4.00%	0.792%
4	9.022	967	975	985	rBV	1600160	2554403	13.74%	2.719%
5	10.446	1211	1217	1229	rBV	339525	521442	2.80%	0.555%
6	10.663	1247	1254	1265	rBV	590892	991962	5.33%	1.056%
7	13.128	1665	1673	1679	rBV	3852563	5662644	30.45%	6.027%
8	13.822	1767	1791	1806	rBV2	1059594	4721648	25.39%	5.025%
9	14.498	1900	1906	1913	rBV	849985	1270740	6.83%	1.352%
10	15.322	2041	2046	2055	rVB	214929	337111	1.81%	0.359%
11	15.881	2135	2141	2150	rVB	785267	1314012	7.07%	1.399%
12	15.992	2154	2160	2167	rVB	3175694	4598651	24.73%	4.894%
13	16.357	2215	2222	2236	rVB	108514	426585	2.29%	0.454%
14	16.639	2264	2270	2272	rBV4	133310	226203	1.22%	0.241%
15	16.733	2281	2286	2296	rVB3	157351	362813	1.95%	0.386%
16	17.004	2321	2332	2356	rBV2	1688131	5226725	28.11%	5.563%
17	17.257	2369	2375	2382	rBV	1059340	1596980	8.59%	1.700%
18	18.157	2522	2528	2535	rBV	1384436	1966025	10.57%	2.092%
19	18.216	2535	2538	2547	rVB	284907	395140	2.12%	0.421%
20	18.457	2575	2579	2591	rVB	376234	608410	3.27%	0.648%
21	19.386	2733	2737	2749	rBV	659004	939076	5.05%	0.999%
22	19.821	2805	2811	2816	rBV	7031261	8669925	46.62%	9.228%
23	19.927	2820	2829	2836	rBV	2918566	6522838	35.08%	6.942%
24	20.010	2836	2843	2848	rBV	4076553	7753292	41.69%	8.252%
25	20.080	2848	2855	2861	rVB	11705558	18595733	100.00%	19.792%
26	20.186	2867	2873	2888	rVB	912045	1512081	8.13%	1.609%
27	20.316	2891	2895	2899	rBV	178185	261004	1.40%	0.278%
28	20.674	2952	2956	2965	rVB	283190	402986	2.17%	0.429%
29	21.057	3018	3021	3027	rBV2	379331	534104	2.87%	0.568%
30	21.245	3049	3053	3061	rBV2	413913	649549	3.49%	0.691%
31	21.345	3065	3070	3076	rBV	1584663	1997548	10.74%	2.126%
32	21.821	3148	3151	3158	rVB	384791	519205	2.79%	0.553%
33	21.963	3171	3175	3188	rVB3	297685	628380	3.38%	0.669%
34	22.433	3251	3255	3260	rBV	324270	478364	2.57%	0.509%
35	23.762	3474	3481	3491	rVB2	1110434	2359420	12.69%	2.511%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

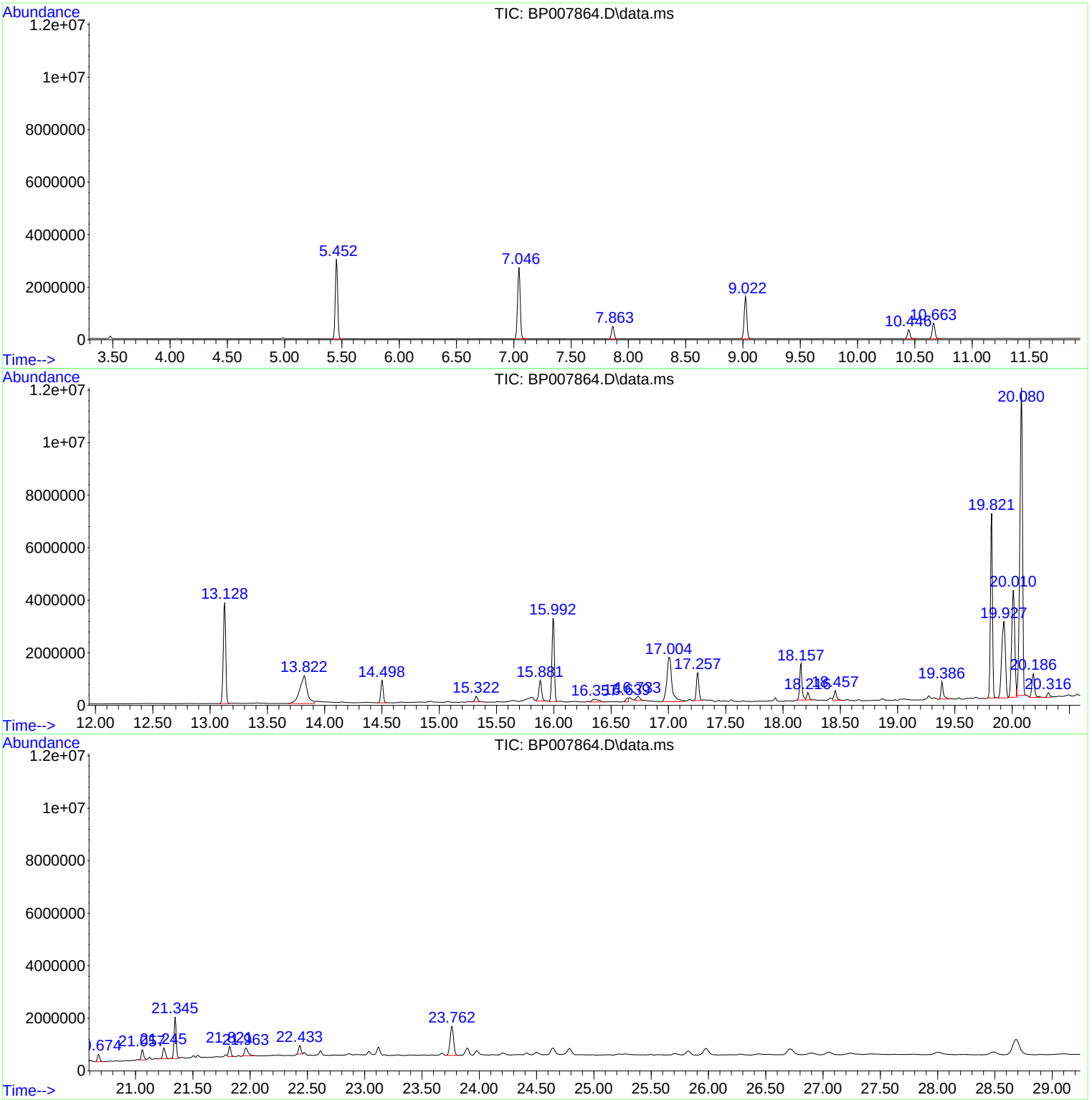
Sum of corrected areas: 93956804

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

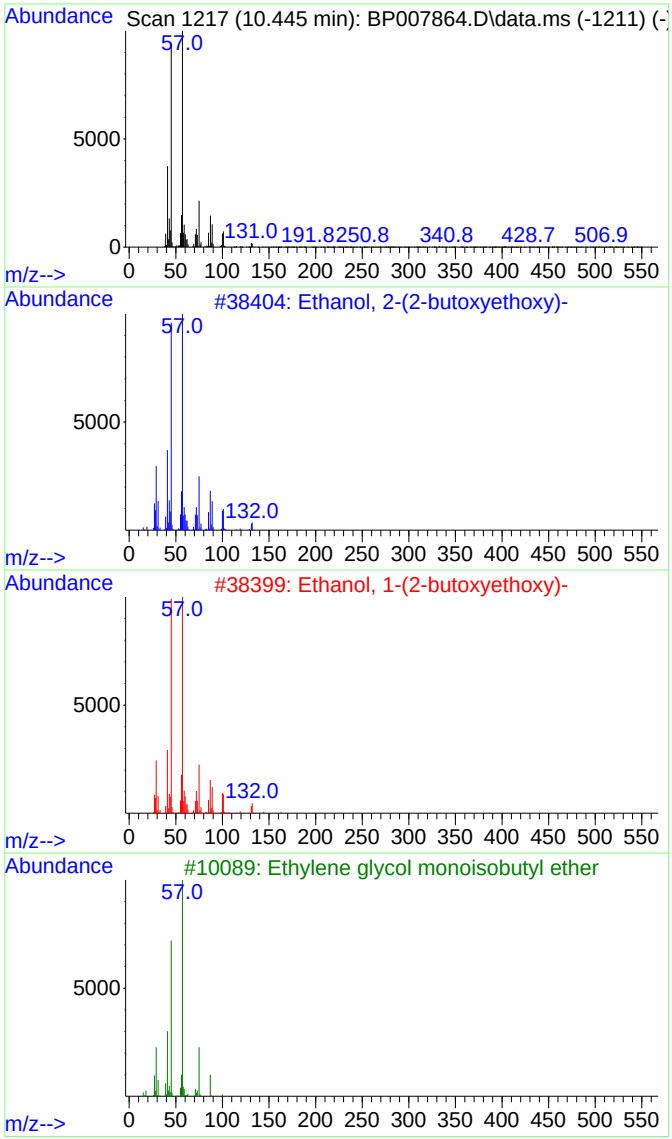
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

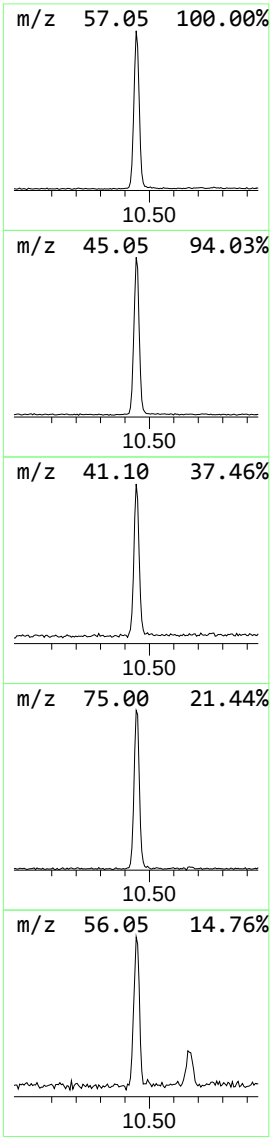
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	10.51 ng	521442	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	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	Hexaethylene glycol	282	C12H26O7	002615-15-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

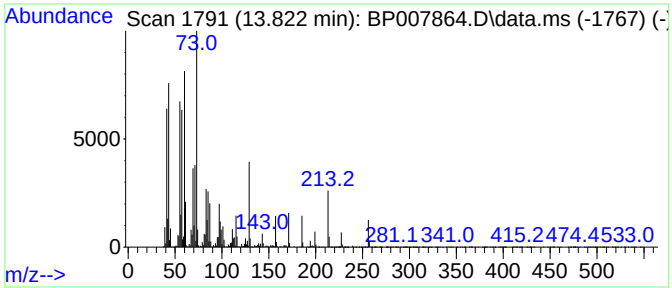
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

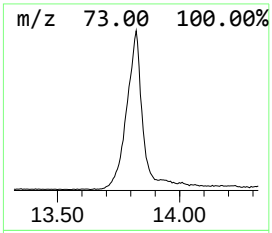
****

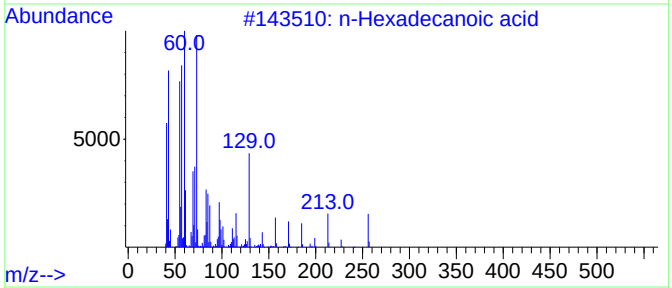
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

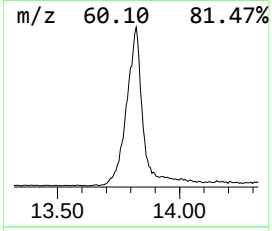
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	74.31 ng	4721650	Acenaphthene-d10	14.504

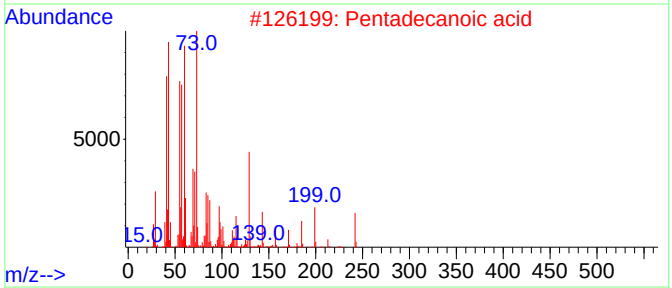
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68

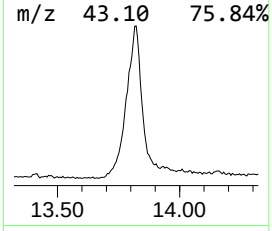


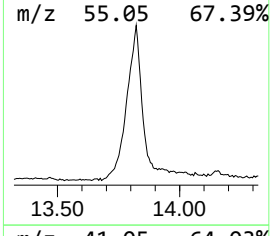


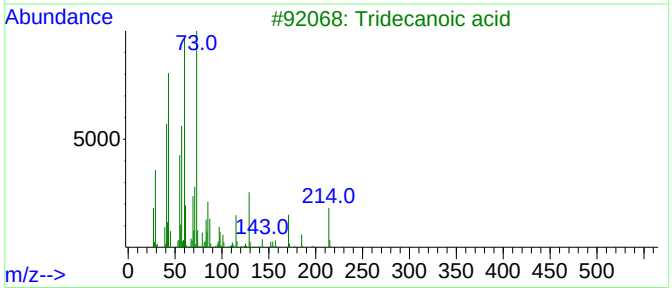


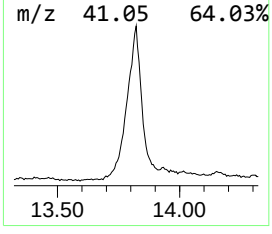












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

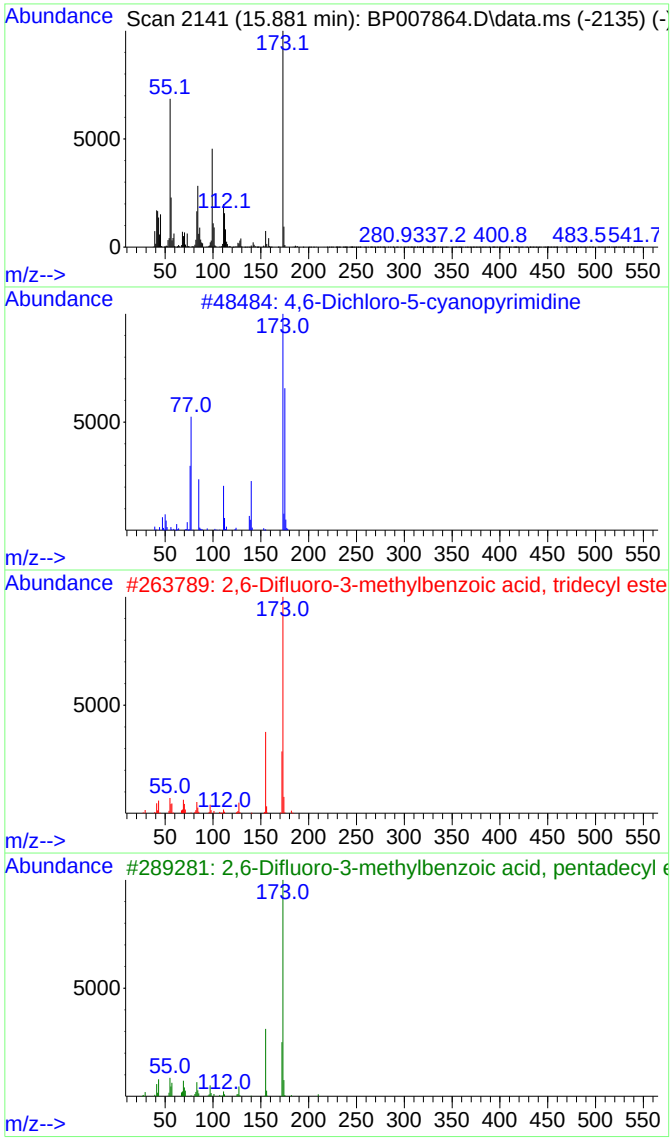
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

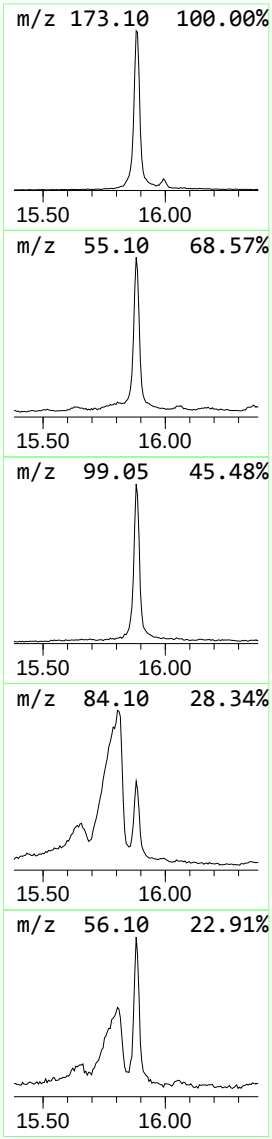
****

Peak Number 3 unknown15.881 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.881	16.46 ng	1314010	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Dichloro-5-cyanopyrimidine	173	C5HCl2N3	005305-45-3	43
2	2,6-Difluoro-3-methylbenzoic aci...	354	C21H32F2O2	1000338-85-0	32
3	2,6-Difluoro-3-methylbenzoic aci...	382	C23H36F2O2	1000338-85-2	23
4	2,6-Difluoro-3-methylbenzoic aci...	396	C24H38F2O2	1000338-85-3	17
5	2,6-Difluoro-3-methylbenzoic aci...	368	C22H34F2O2	1010338-85-1	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

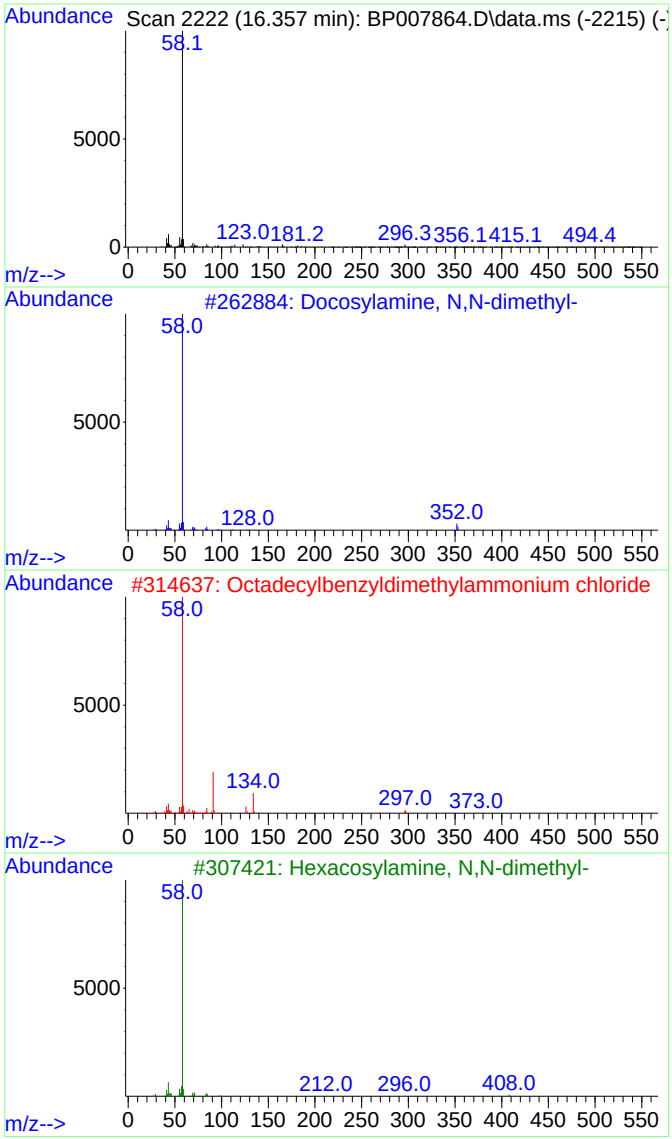
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

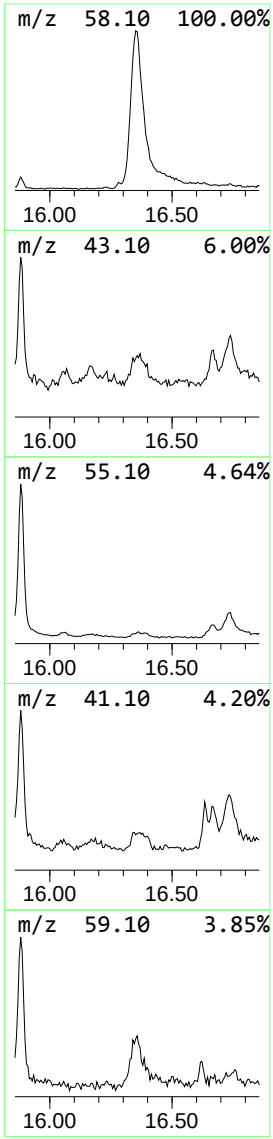
****

Peak Number 4 Docosylamine, N,N-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.357	5.34 ng	426585	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosylamine, N,N-dimethyl-	353	C24H51N	1000406-30-6	72
2	Octadecylbenzyldimethylammonium ...	423	C27H50ClN	000122-19-0	72
3	Hexacosylamine, N,N-dimethyl-	409	C28H59N	1000406-30-8	64
4	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	64
5	1-Nonadecanamine, N,N-dimethyl-	311	C21H45N	049859-87-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

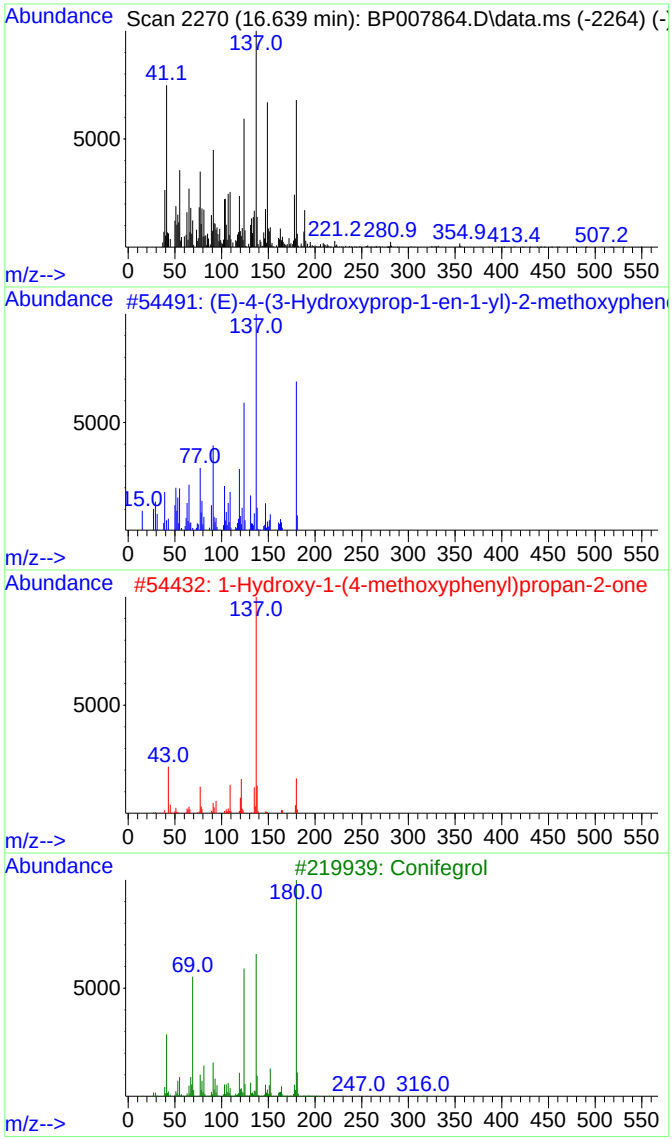
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

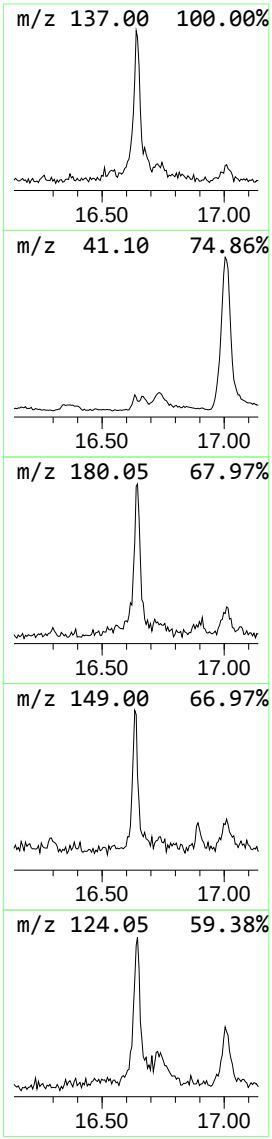
****

Peak Number 5 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.639	2.83 ng	226203	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	64
2	1-Hydroxy-1-(4-methoxyphenyl)pro...	180	C10H12O3	015482-29-8	38
3	Conifegrol	316	C20H28O3	129350-09-0	35
4	3,6-Dimethyl-2,3,3a,4,5,7a-hexah...	152	C10H16O	070786-44-6	25
5	Propenoic acid, 3-(2-thienyl)-, ...	464	C13H7Br3O2S	284665-05-0	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

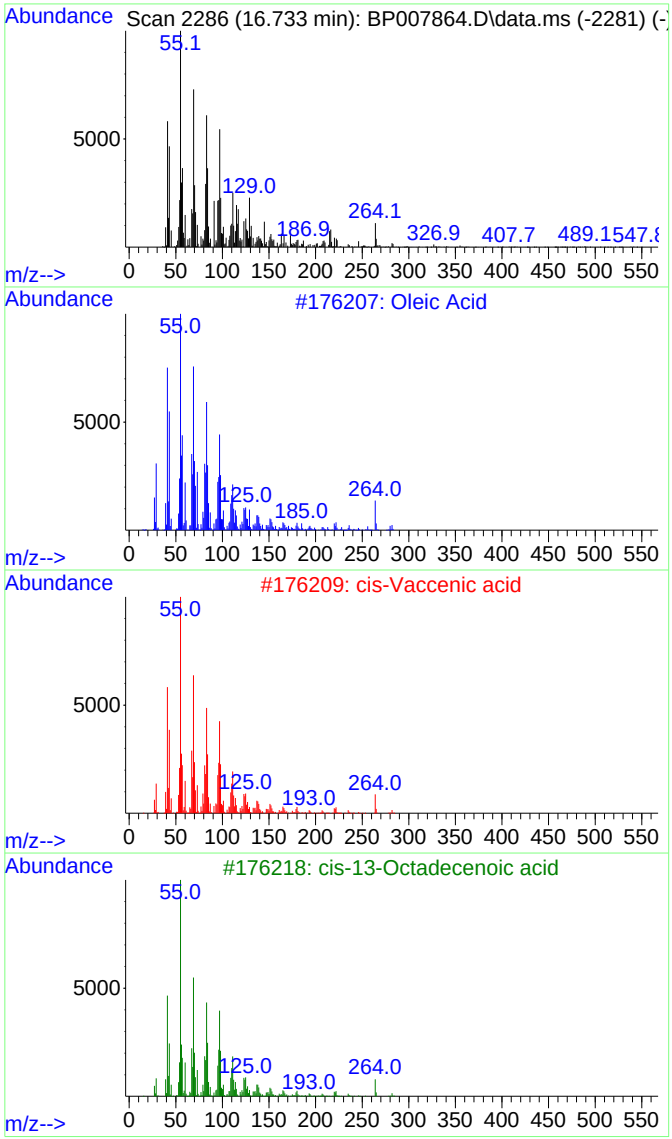
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

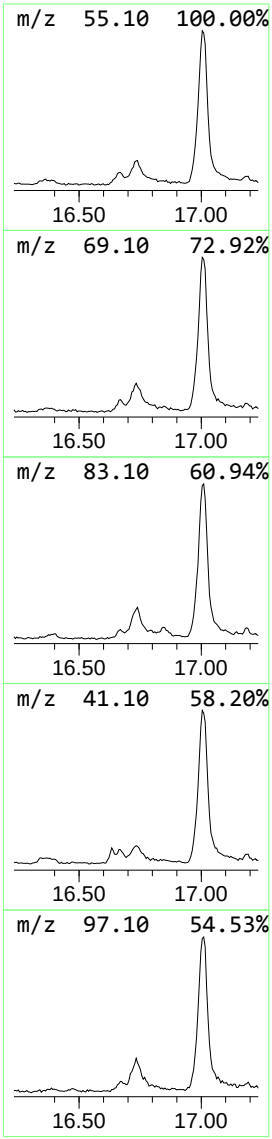
****

Peak Number 6 Oleic Acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	4.54 ng	362813	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	93
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	93
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	89
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

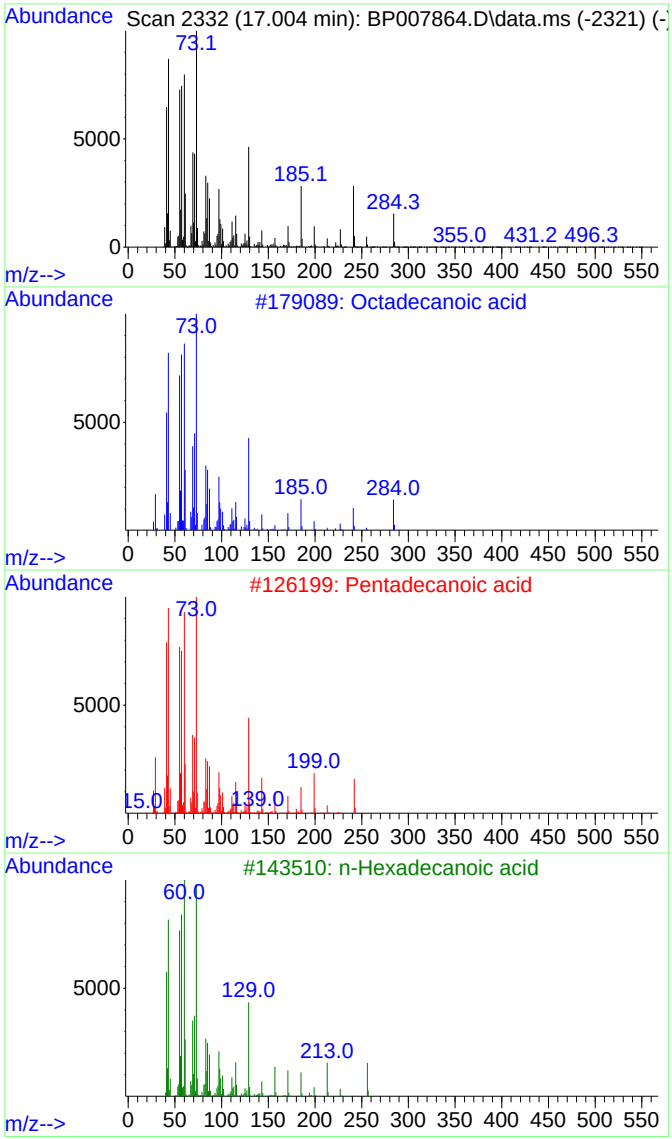
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

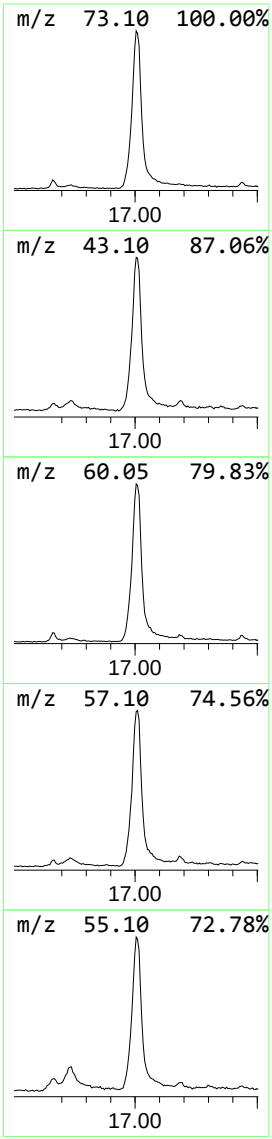
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.004	65.46 ng	5226730	Phenanthrene-d10	17.257

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-10-4.5-5.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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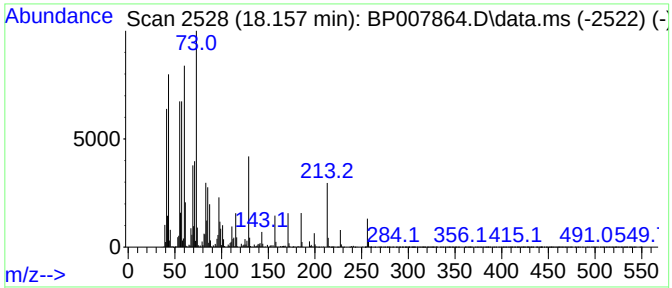
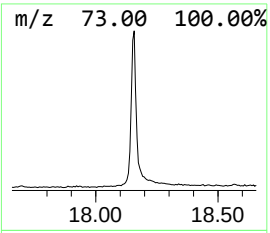
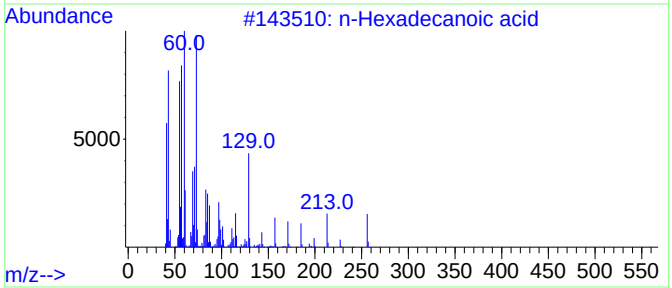
Peak Number 8 Tridecanoic acid Concentration Rank 6

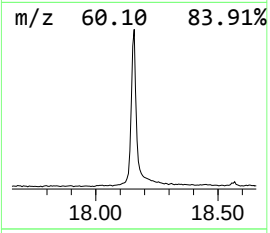
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	24.62 ng	1966030	Phenanthrene-d10	17.257

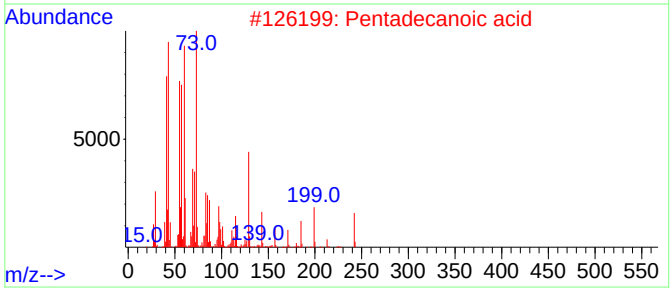
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Undecanoic acid	186	C11H22O2	000112-37-8	87

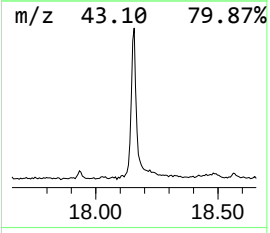


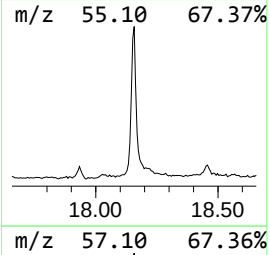


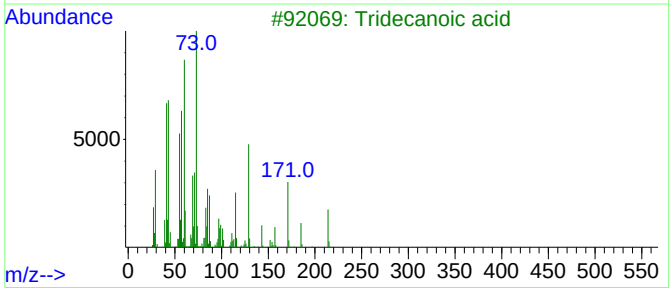


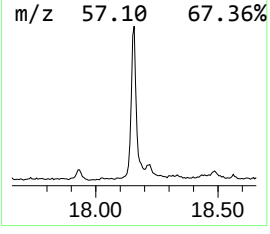












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Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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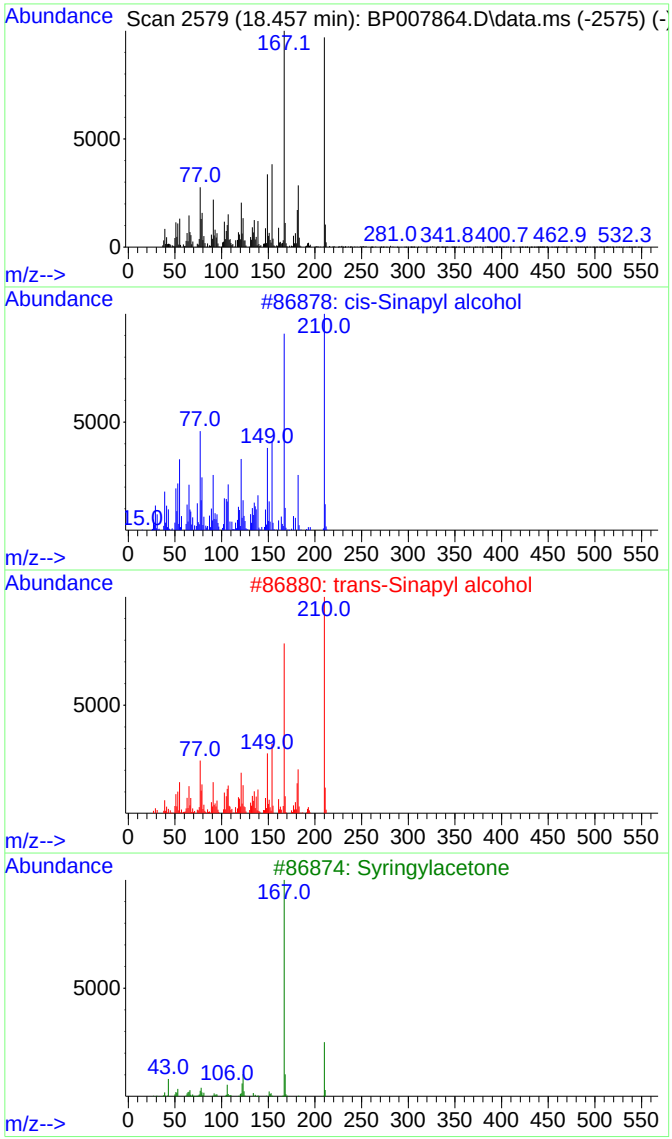
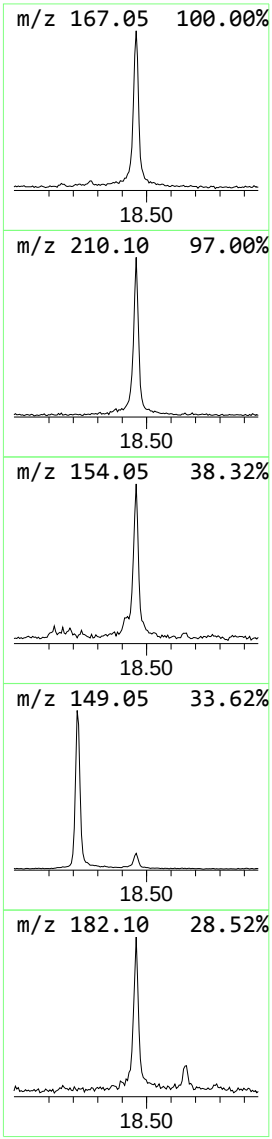
Peak Number 9 cis-Sinapyl alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.457	7.62 ng	608410	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	95
2	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	94
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	1-(1-Hydroxybutyl)-2,5-dimethoxy...	210	C12H18O3	149083-03-4	58
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	55





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Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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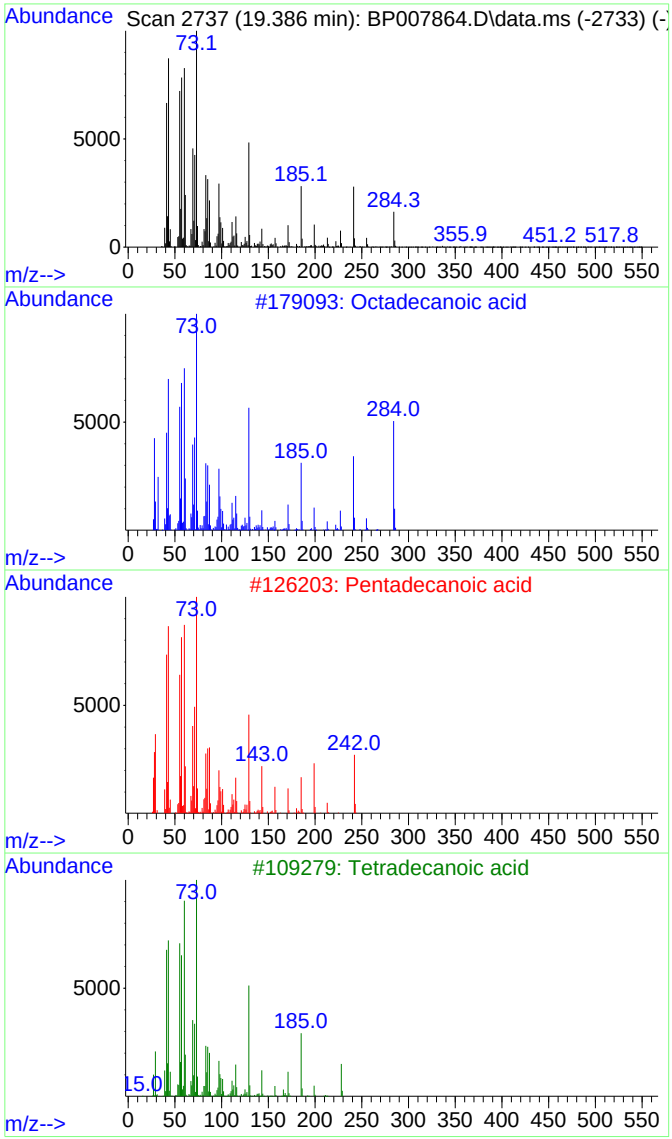
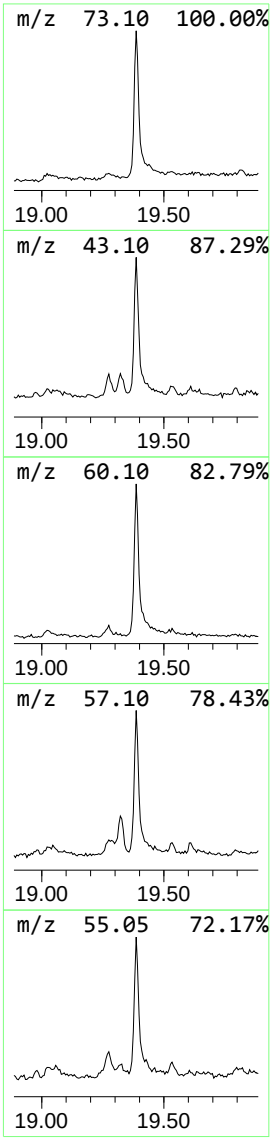
Peak Number 10 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	9.40 ng	939076	Chrysene-d12	21.345

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-10-4.5-5.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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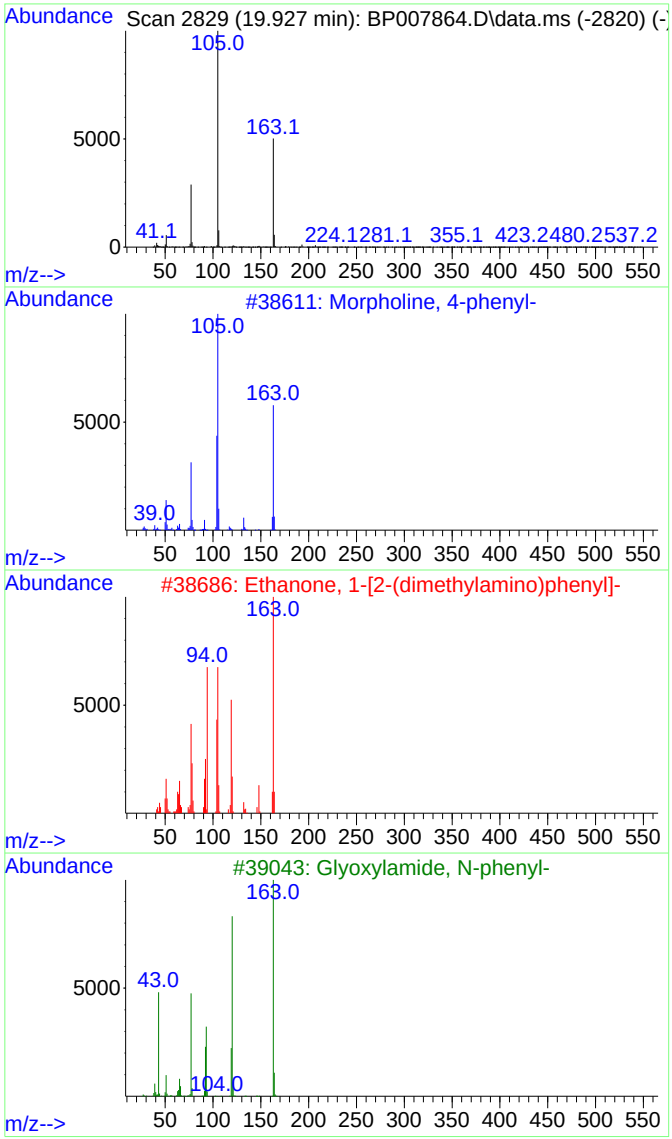
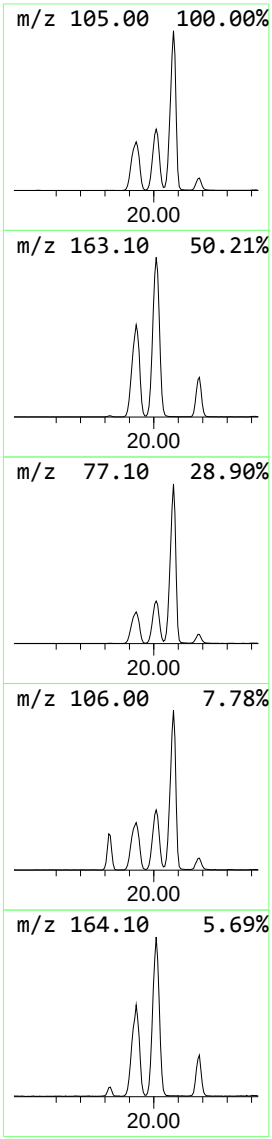
Peak Number 11 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.927	65.31 ng	6522840	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	56
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	43
5	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	43





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Misc :
ALS Vial : 4 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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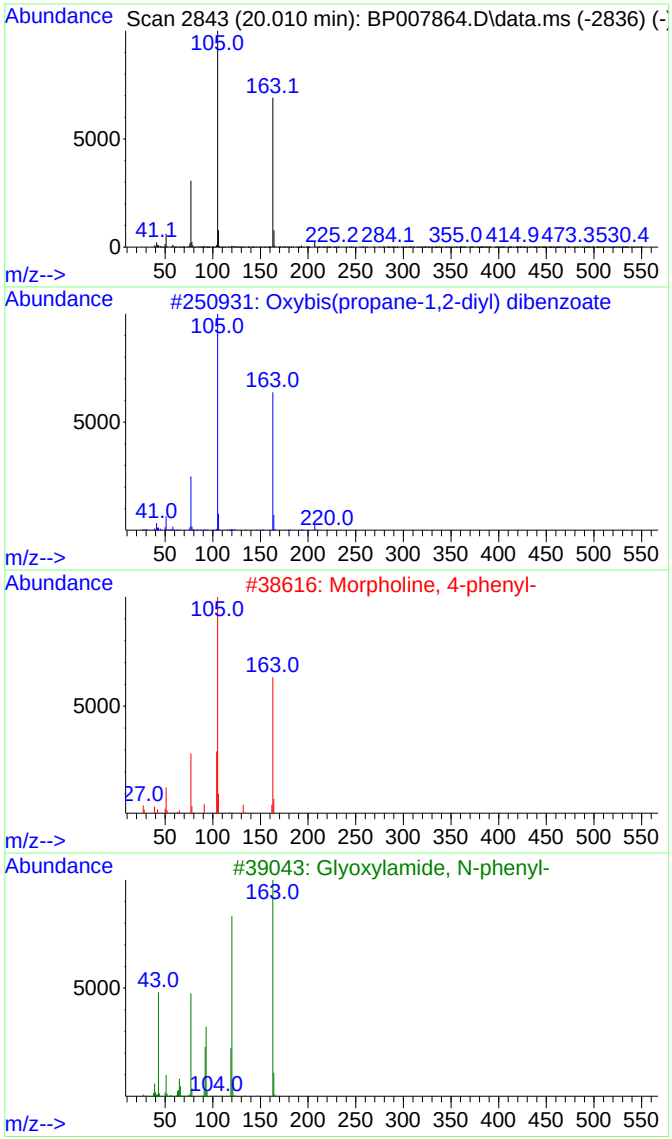
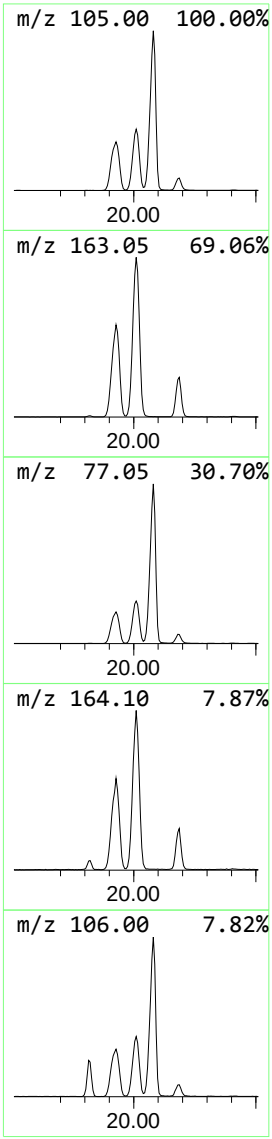
Peak Number 12 Glyoxylamide, N-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.010	77.63 ng	7753290	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	83
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	Phenylglyoxylic acid, isopropyl ...	192	C11H12O3	1000453-46-3	43
5	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43





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Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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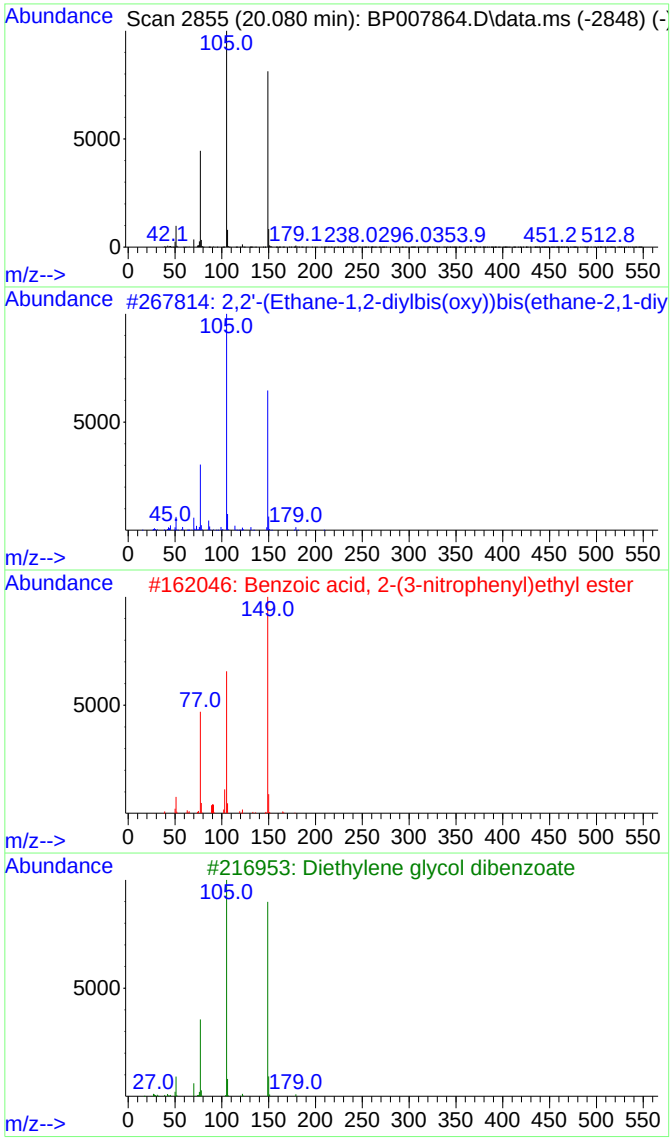
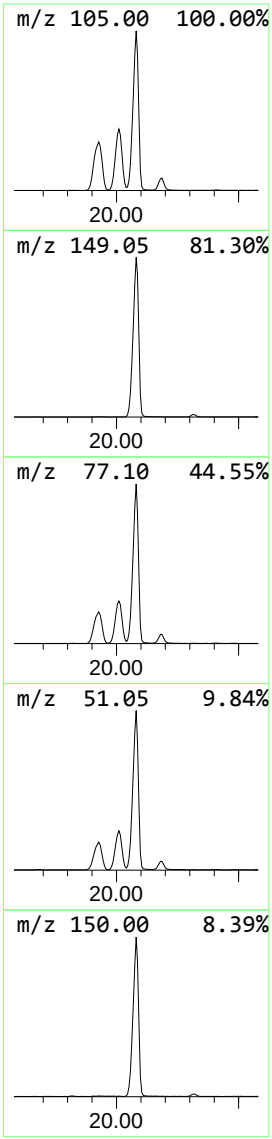
Peak Number 13 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.080	186.19 ng	18595700	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	64
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59





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Sample : M4579-02
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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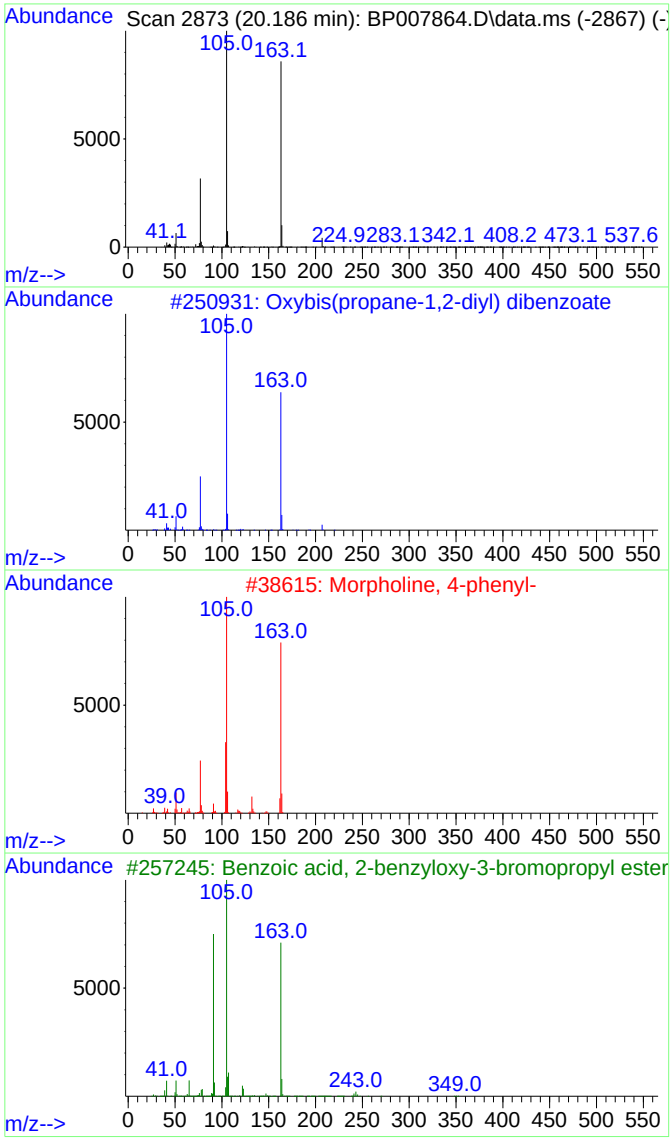
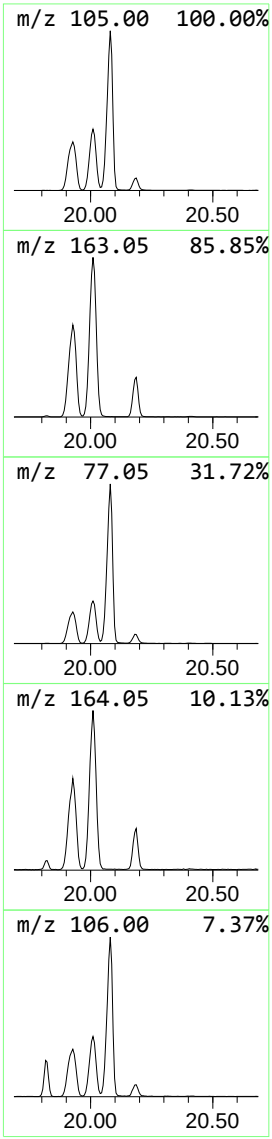
Peak Number 14 Oxybis(propane-1,2-diyl) di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.186	15.14 ng	1512080	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	90
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	59
4	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
5	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	43





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Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-10-4.5-5.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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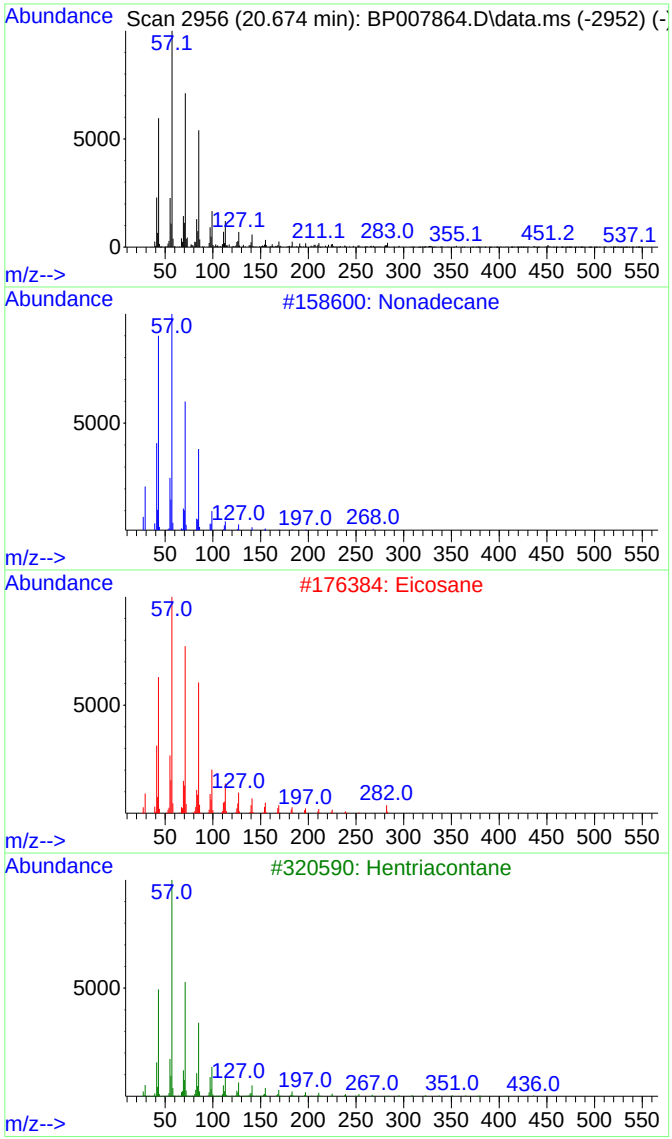
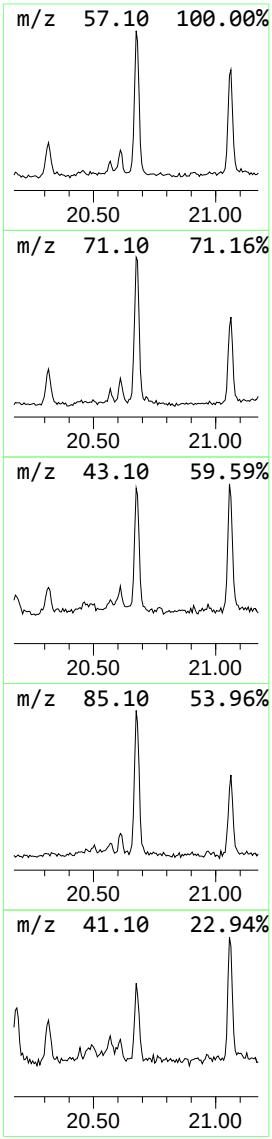
Peak Number 15 Nonadecane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.674	4.03 ng	402986	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	98
2	Eicosane	282	C20H42	000112-95-8	93
3	Hentriacontane	437	C31H64	000630-04-6	93
4	Dotriacontane	451	C32H66	000544-85-4	91
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	90





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ALS Vial : 4 Sample Multiplier: 1

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SB-10-4.5-5.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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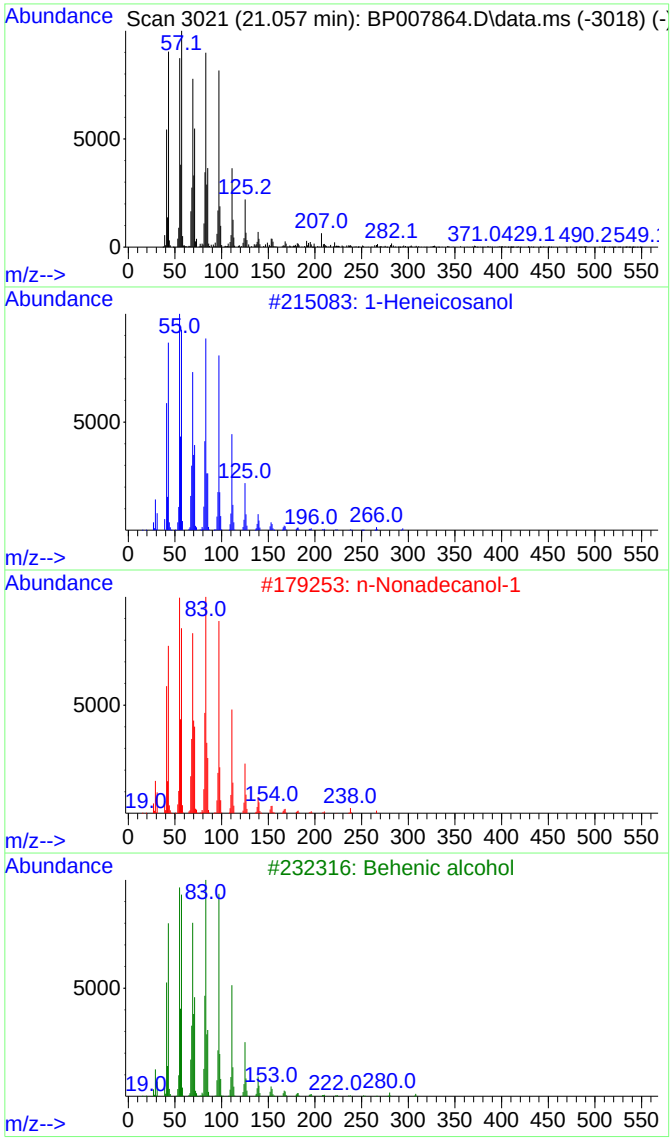
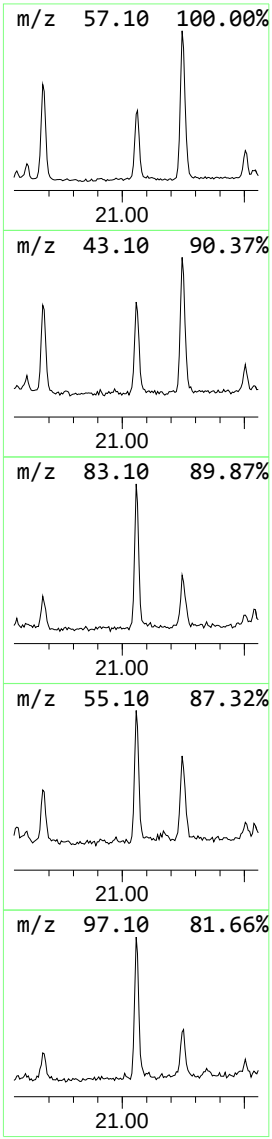
Peak Number 16 1-Heneicosanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	5.35 ng	534104	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





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ALS Vial : 4 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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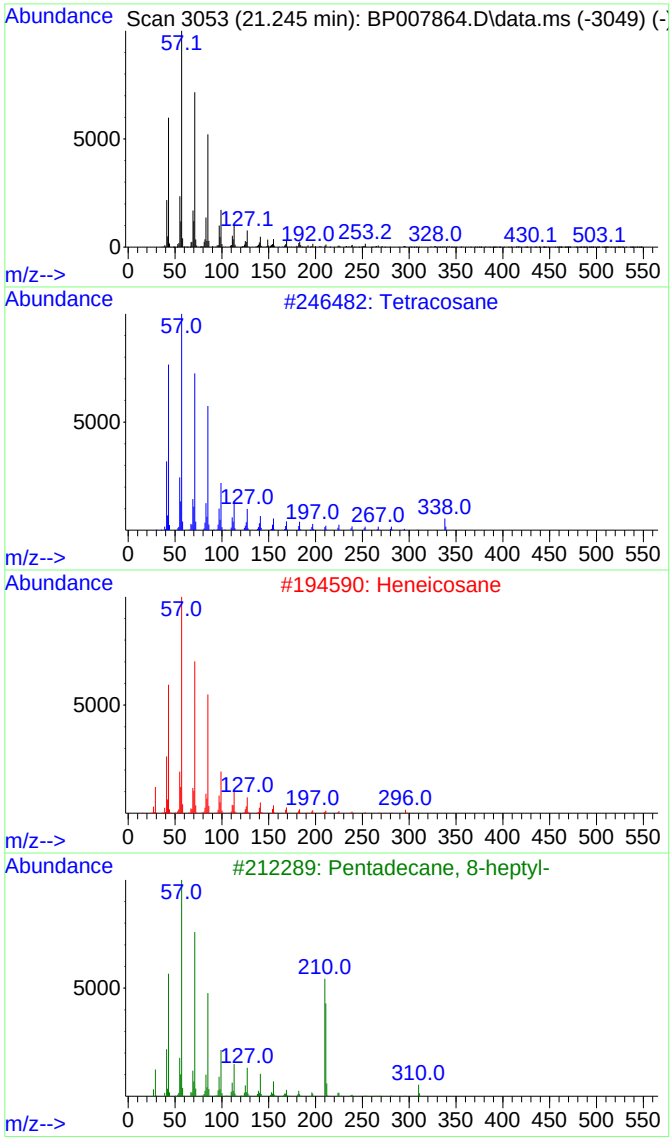
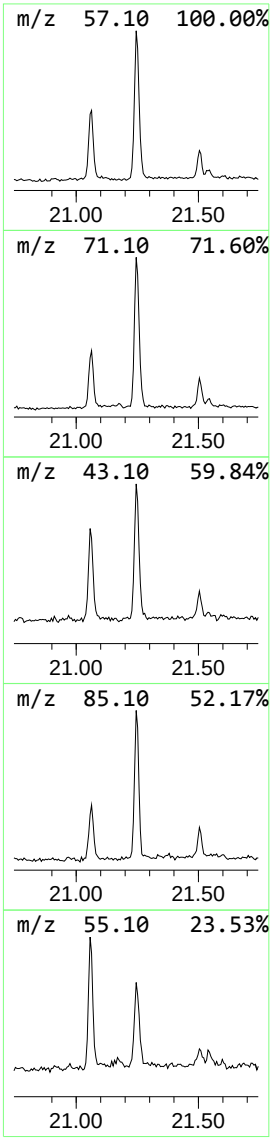
Peak Number 17 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	6.50 ng	649549	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Heneicosane	296	C21H44	000629-94-7	93
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	93
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
5	Nonadecane	268	C19H40	000629-92-5	93





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Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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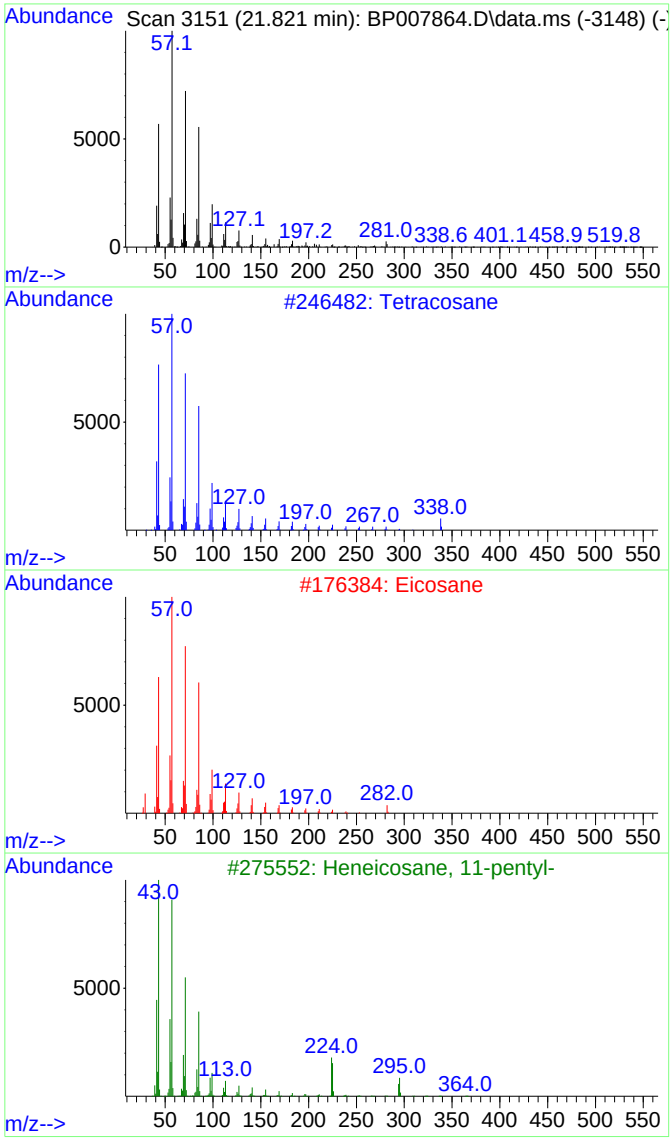
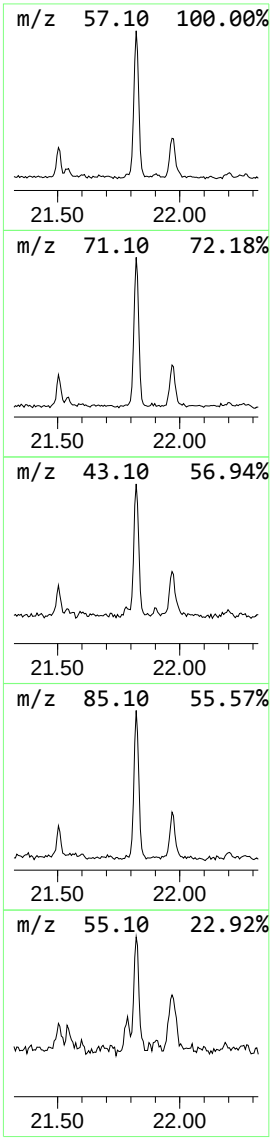
Peak Number 18 Tetracosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.821	5.20 ng	519205	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Eicosane	282	C20H42	000112-95-8	93
3	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





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Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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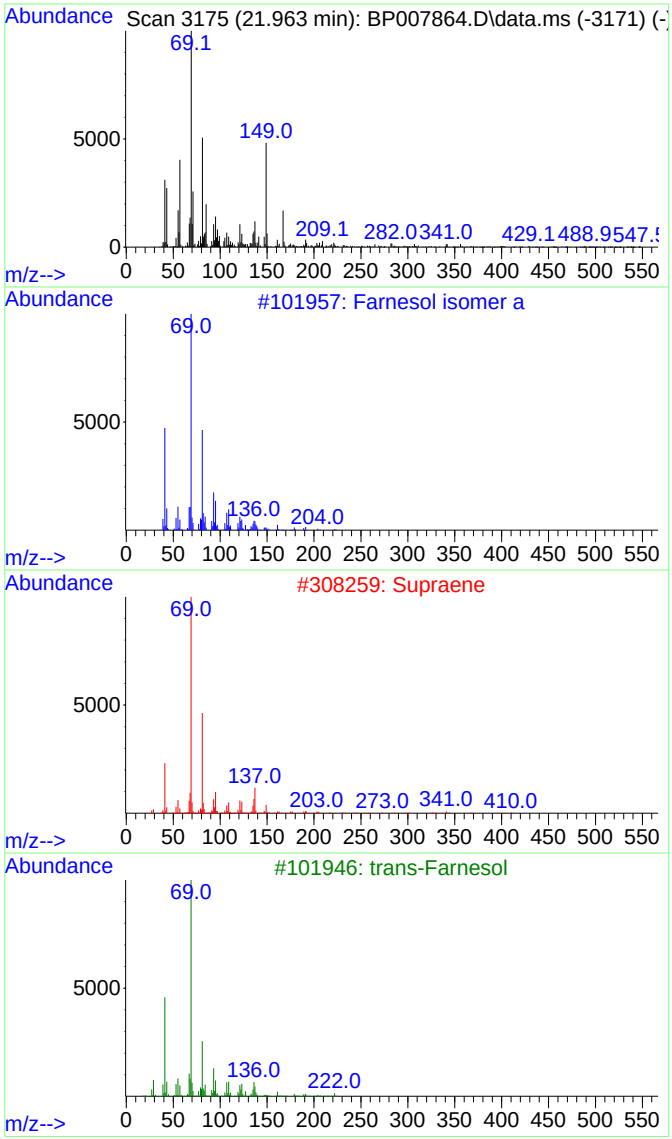
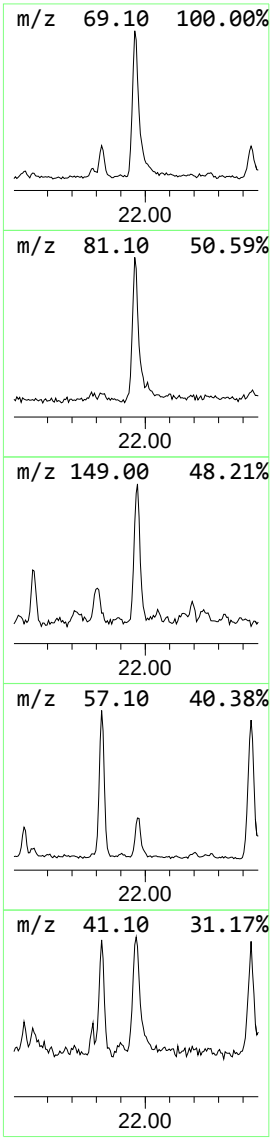
Peak Number 19 Farnesol isomer a Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.962	6.29 ng	628380	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	50
2	Supraene	410	C30H50	007683-64-9	49
3	trans-Farnesol	222	C15H26O	000106-28-5	46
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	45
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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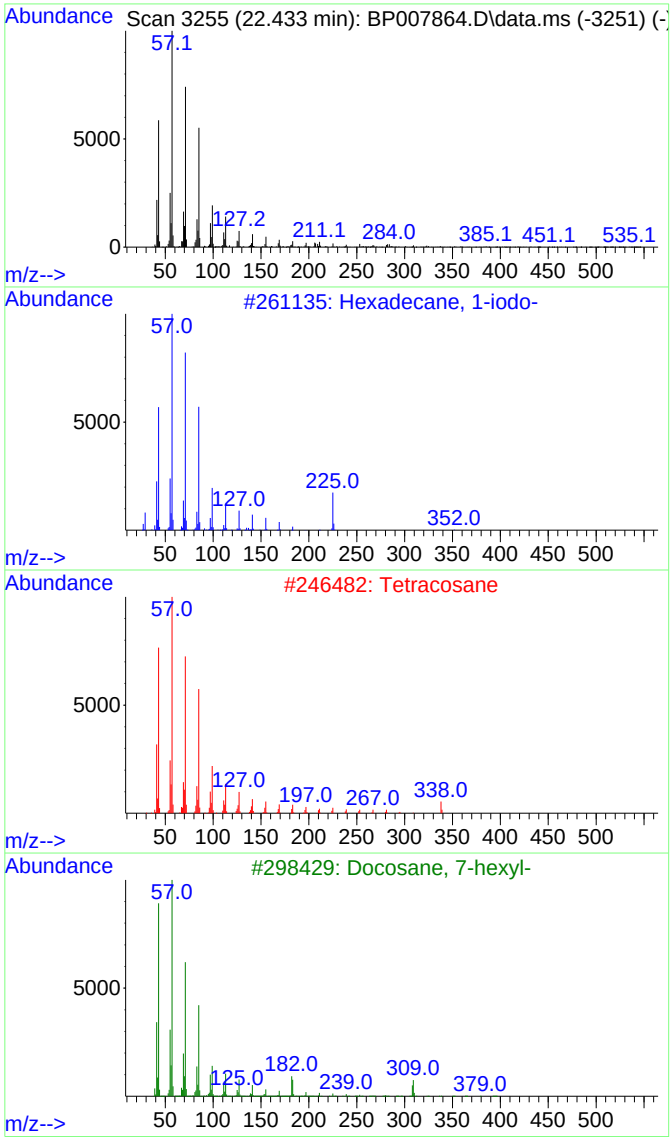
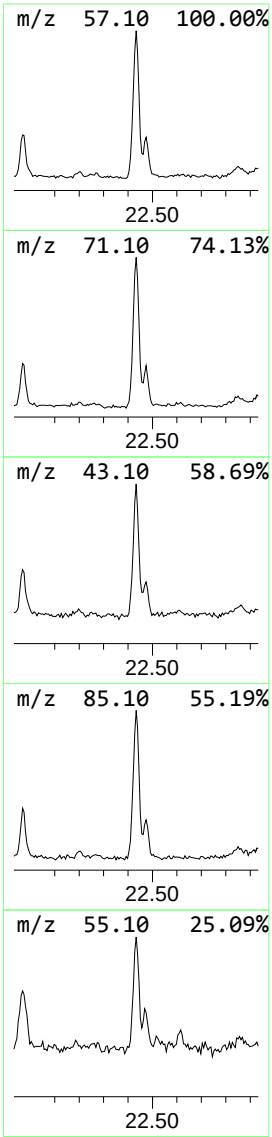
Peak Number 20 Hexadecane, 1-iodo- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.433	4.79 ng	478364	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	96
2	Tetracosane	338	C24H50	000646-31-1	95
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
4	2-Methyltetracosane	352	C25H52	001560-78-7	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110821\
Data File : BP007864.D
Acq On : 08 Nov 2021 17:00
Operator : CG/JU
Sample : M4579-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-10-4.5-5.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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...	10.445	10.5	ng	521442	2	10.663	991962	20.0
n-Hexadecanoic ...	13.822	74.3	ng	4721650	3	14.504	1270740	20.0
unknown15.881	15.881	16.5	ng	1314010	4	17.257	1596980	20.0
Docosylamine, N...	16.357	5.3	ng	426585	4	17.257	1596980	20.0
(E)-4-(3-Hydrox...	16.639	2.8	ng	226203	4	17.257	1596980	20.0
Oleic Acid	16.733	4.5	ng	362813	4	17.257	1596980	20.0
Octadecanoic acid	17.004	65.5	ng	5226730	4	17.257	1596980	20.0
Tridecanoic acid	18.157	24.6	ng	1966030	4	17.257	1596980	20.0
cis-Sinapyl alc...	18.457	7.6	ng	608410	4	17.257	1596980	20.0
Pentadecanoic acid	19.386	9.4	ng	939076	5	21.345	1997550	20.0
Morpholine, 4-p...	19.927	65.3	ng	6522840	5	21.345	1997550	20.0
Glyoxylamide, N...	20.010	77.6	ng	7753290	5	21.345	1997550	20.0
2,2'-(Ethane-1,...	20.080	186.2	ng	18595700	5	21.345	1997550	20.0
Oxybis(propane-...	20.186	15.1	ng	1512080	5	21.345	1997550	20.0
Nonadecane	20.674	4.0	ng	402986	5	21.345	1997550	20.0
1-Heneicosanol	21.057	5.3	ng	534104	5	21.345	1997550	20.0
Heneicosane	21.245	6.5	ng	649549	5	21.345	1997550	20.0
Tetracosane	21.821	5.2	ng	519205	5	21.345	1997550	20.0
Farnesol isomer a	21.962	6.3	ng	628380	5	21.345	1997550	20.0
Hexadecane, 1-i...	22.433	4.8	ng	478364	5	21.345	1997550	20.0