LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-45A

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008228.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.387	401	408	415	rBV	541209	823216	3.92%	1.318%
2	6.981	667	679	690	rBV	301399	522432	2.49%	0.836%
3	7.787	810	816	825	rVB	267148	410710	1.96%	0.657%
4	8.952	1007	1014	1026	rVB	855278	1414536	6.74%	2.264%
5	10.587	1284	1292	1300	rBV	321695	535433	2.55%	0.857%
6	13.057	1705	1712	1719	rBV	1954913	2938217	14.00%	4.703%
7	14.440	1941	1947	1955	rVB	478971	708317	3.38%	1.134%
8	15.939	2196	2202	2210	rVB	1699955	2433576	11.60%	3.896%
9	16.598	2309	2314	2327	rVB3	141071	292075	1.39%	0.468%
10	17.198	2411	2416	2423	rBV	599667	859209	4.10%	1.375%
11	17.551	2457	2476	2491	rBV	1537980	7272403	34.66%	11.641%
12	17.751	2492	2510	2520	rVV2	2020327	8810950	42.00%	14.104%
13	17.939	2520	2542	2555	rVB	5943352	20980306	100.00%	33.584%
14	18.104	2560	2570	2584	rVV2	872469	2234902	10.65%	3.577%
15	18.416	2619	2623	2634	rVB	376471	614490	2.93%	0.984%
16	18.957	2709	2715	2722	rBV	159751	309742	1.48%	0.496%
17	19.339	2776	2780	2793	rVB	378023	526560	2.51%	0.843%
18	19.775	2849	2854	2859	rBV	3609760	4306249	20.53%	6.893%
19	19.904	2870	2876	2883	rVB2	223471	468947	2.24%	0.751%
20	20.680	3003	3008	3015	rVB	294181	488135	2.33%	0.781%
21	21.022	3062	3066	3072	rBV2	226488	375903	1.79%	0.602%
22	21.080	3072	3076	3081	rVB	438242	550910	2.63%	0.882%
23	21.304	3110	3114	3119	rBV	873832	1128482	5.38%	1.806%
24	21.363	3119	3124	3130	rVV	313677	601087	2.87%	0.962%
25	22.063	3239	3243	3251	rVB	237791	476794	2.27%	0.763%
26	22.833	3370	3374	3382	rVB	285589	508279	2.42%	0.814%
27	23.704	3515	3522	3535	rVB3	688631	1879434	8.96%	3.008%

Sum of corrected areas: 62471294

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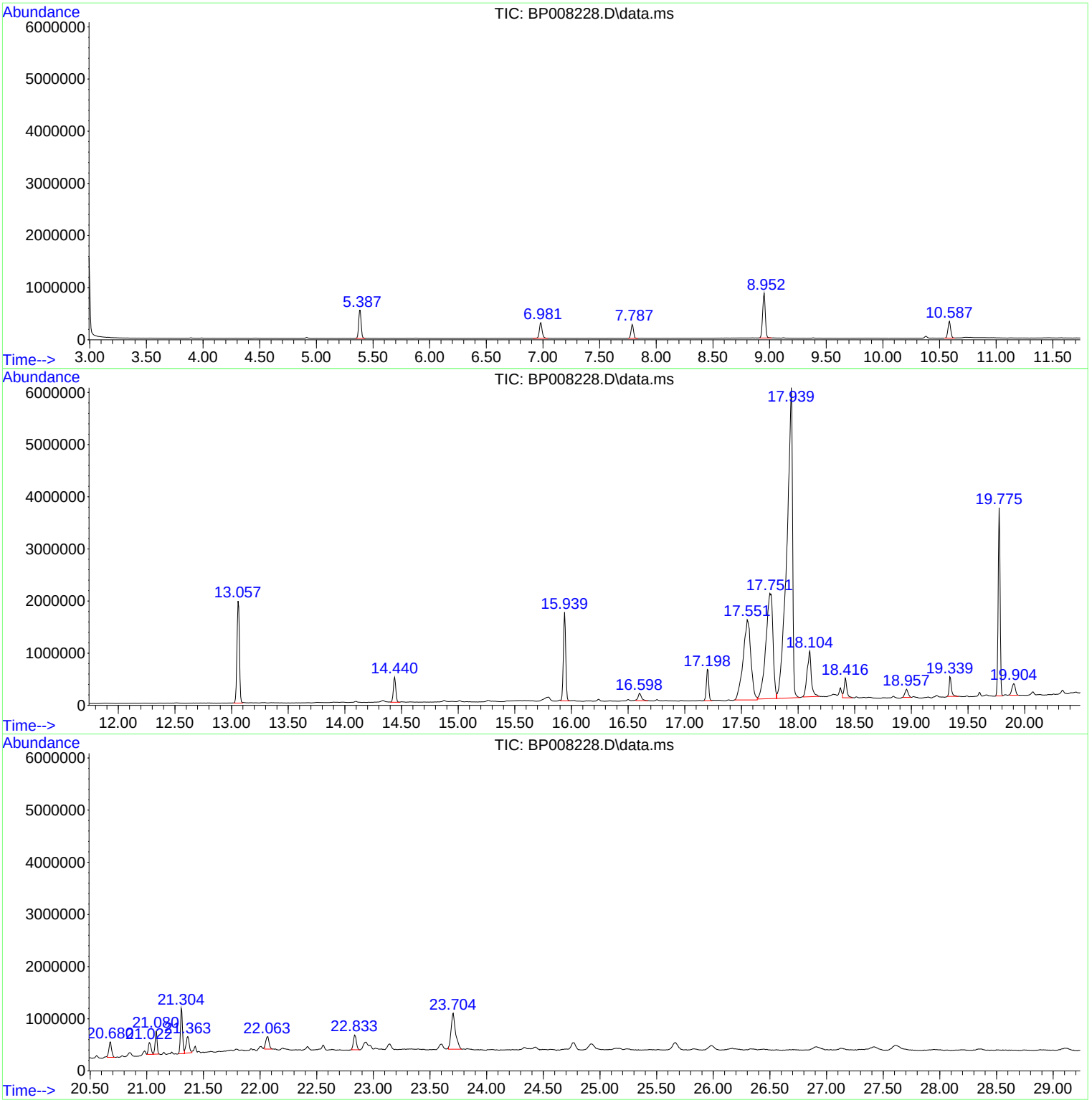
Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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Data File : BP008228.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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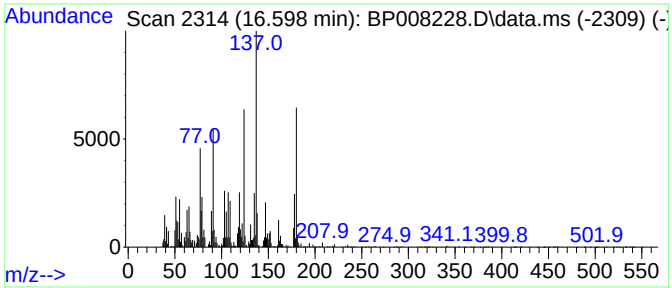
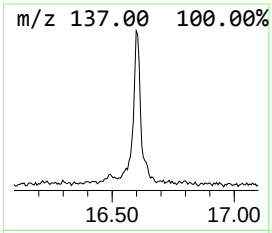
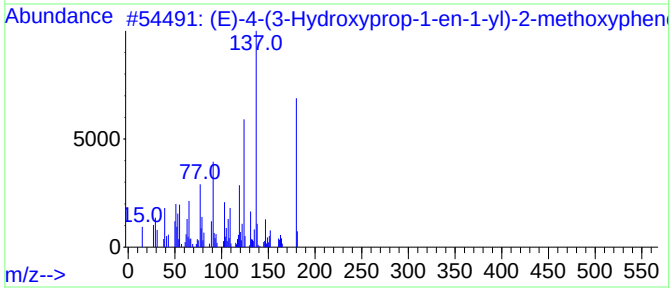
****
Peak Number 1 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 13

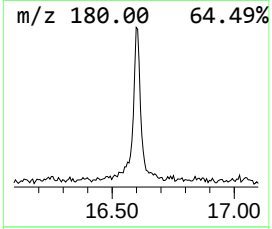
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	6.80 ng	292075	Phenanthrene-d10	17.204

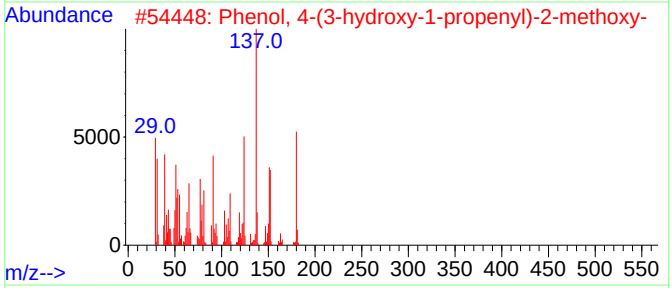
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	58
2	Phenol, 4-(3-hydroxy-1-propenyl)...	180	C10H12O3	000458-35-5	58
3	1-Hydroxy-1-(4-methoxyphenyl)pro...	180	C10H12O3	015482-29-8	43
4	6-Hydroxyeugenol	180	C10H12O3	004055-72-5	35
5	Benzaldehyde, 2-hydroxy-, oxime	137	C7H7NO2	000094-67-7	35

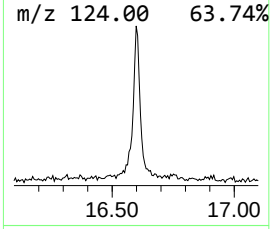


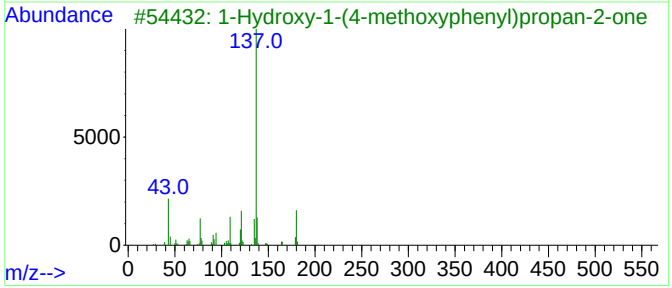


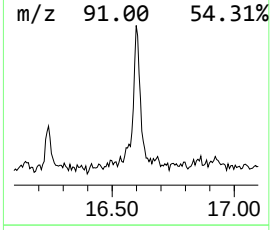


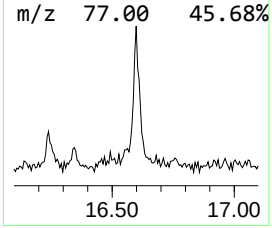












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Acq On : 06 Dec 2021 14:47
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

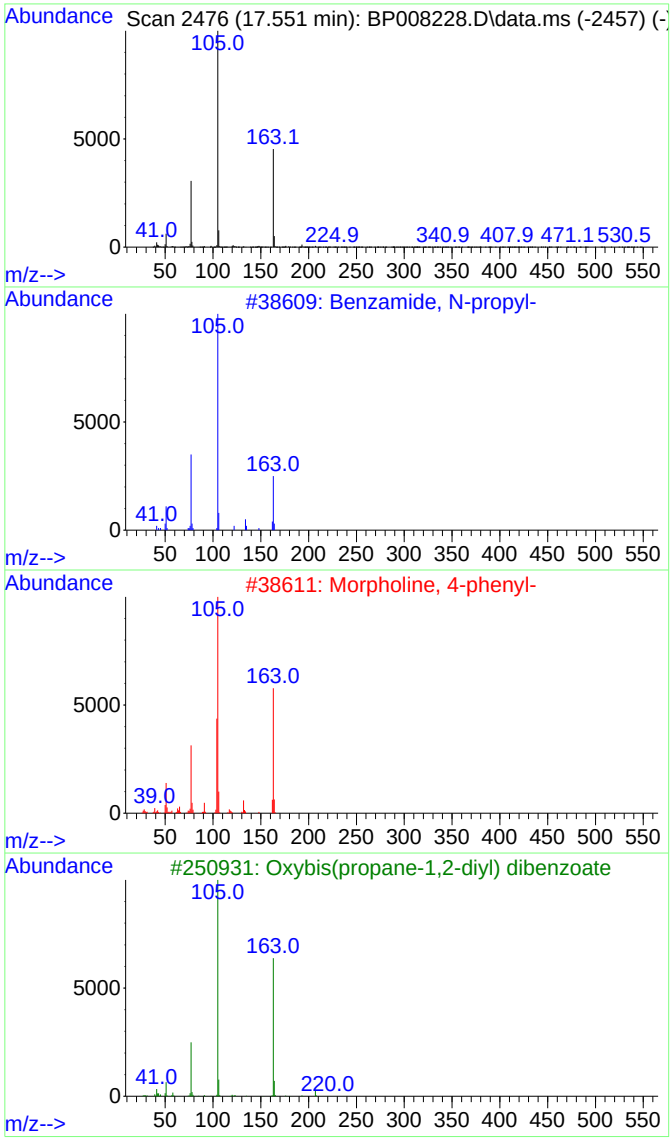
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

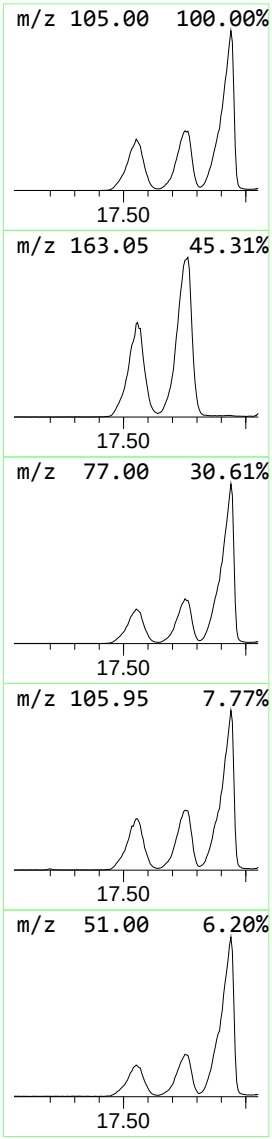
****

Peak Number 2 Benzamide, N-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.551	169.28 ng	7272400	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	56
4	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	38
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	38





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

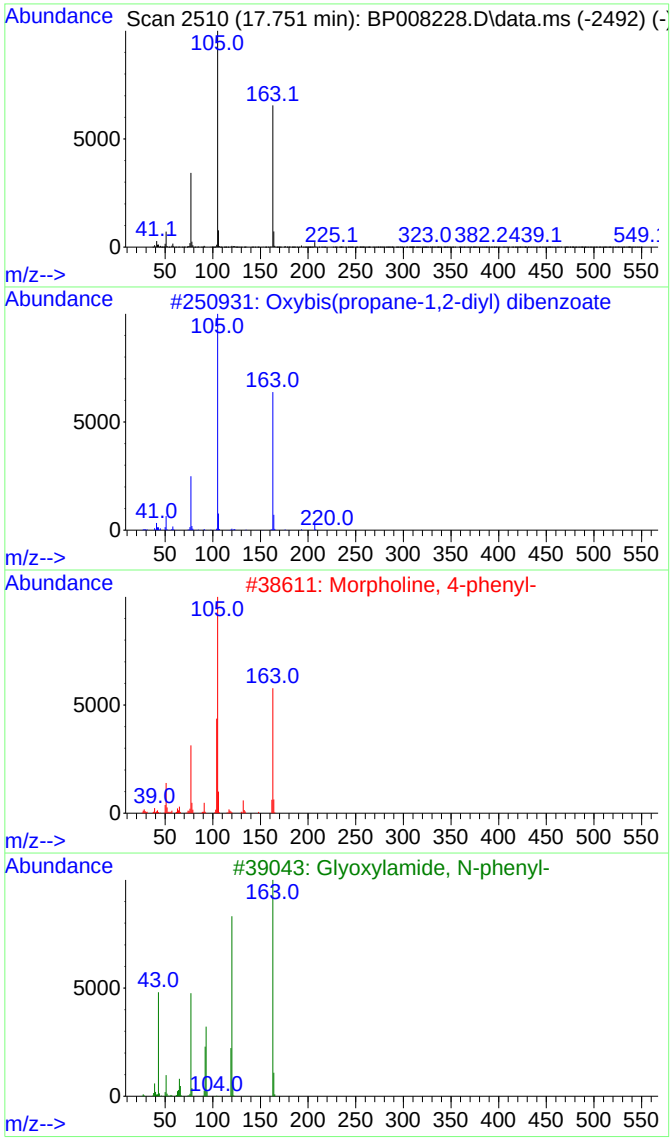
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

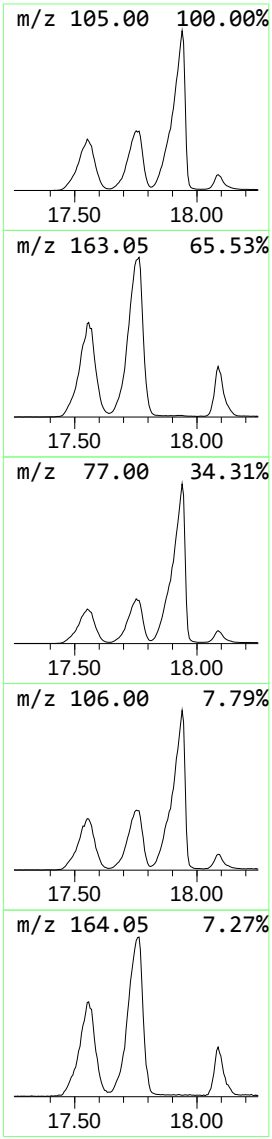
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Oxybis(propane-1,2-diyl) di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.751	205.09 ng	8810950	Phenanthrene-d10	17.204

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	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43
5	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
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Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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TIC Library : C:\Database\NIST20.L
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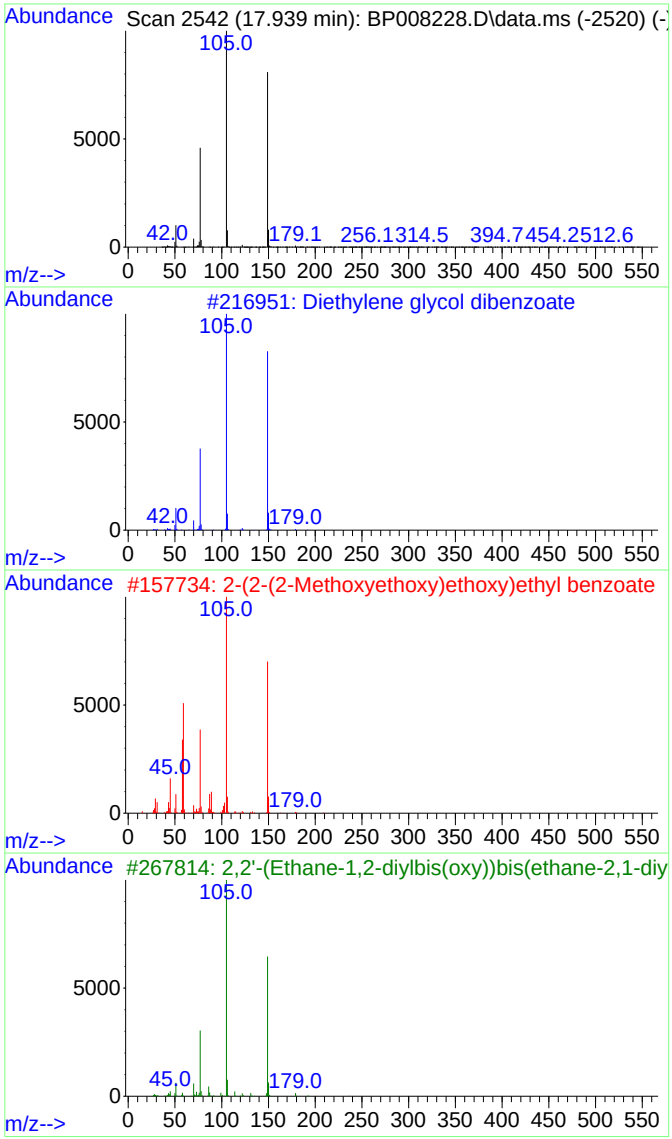
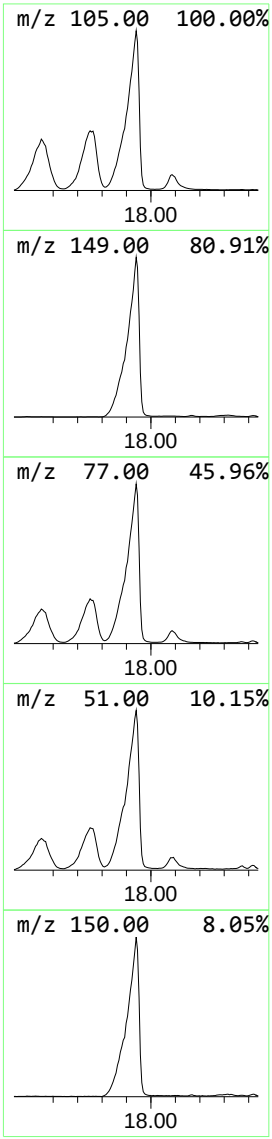
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	488.36 ng	20980300	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72
5	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	64





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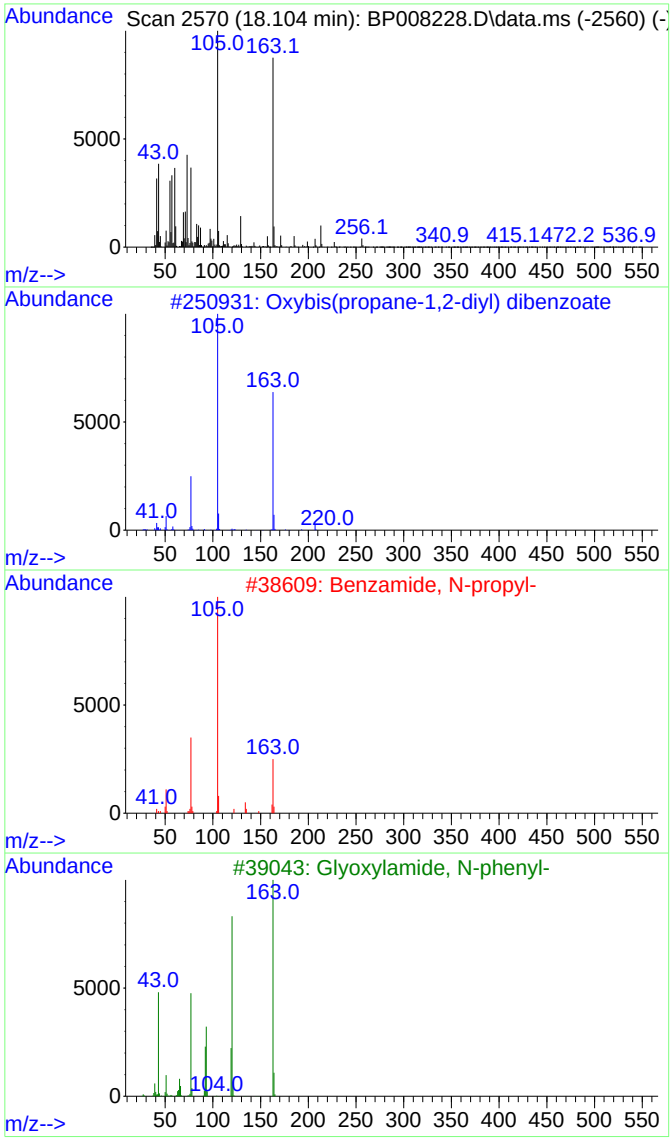
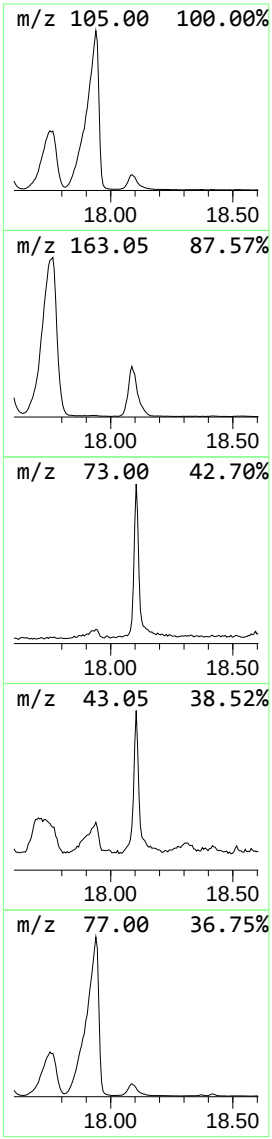
Peak Number 5 unknown18.104 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	52.02 ng	2234900	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	52
2	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	50
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	43
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
5	Phthalic acid, 2-isopropylphenyl...	298	C18H18O4	1000315-52-2	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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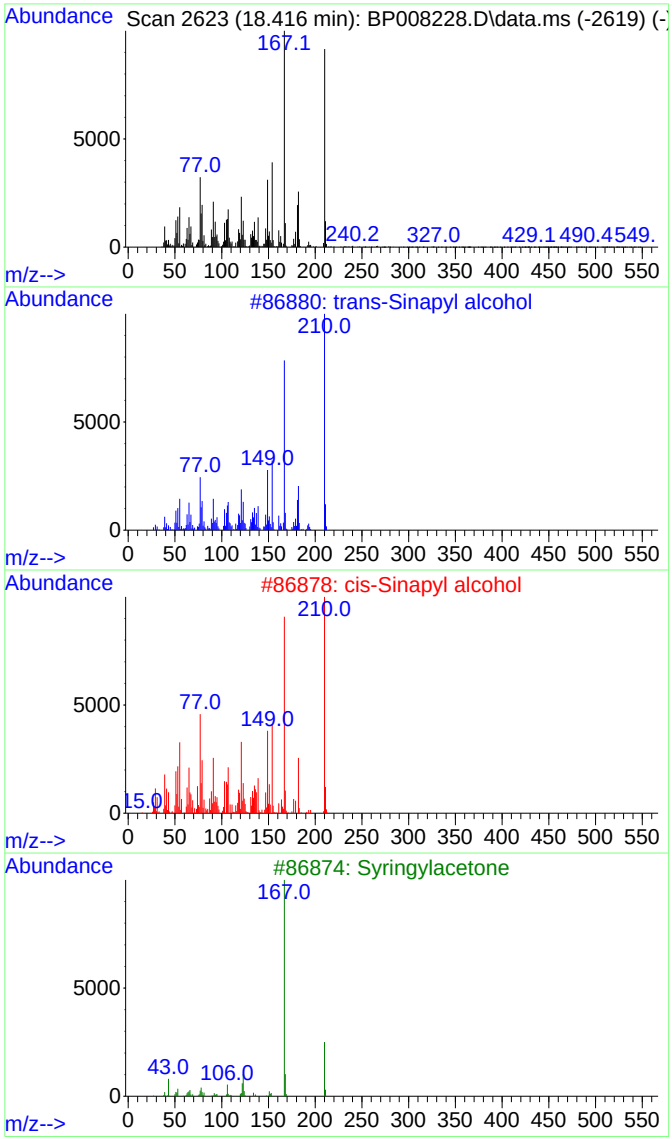
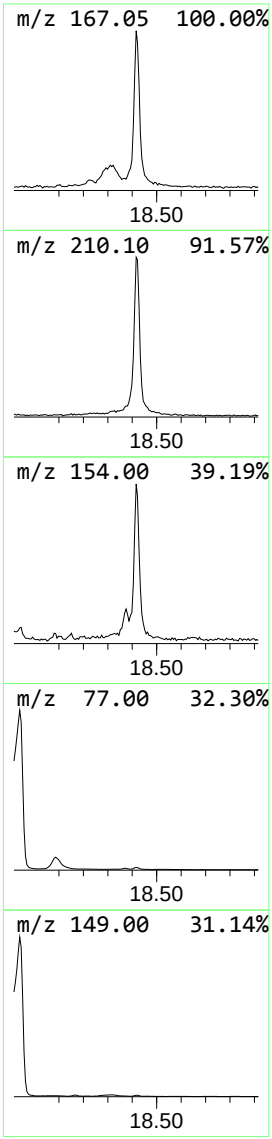
Peak Number 6 trans-Sinapyl alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.416	14.30 ng	614490	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	93
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	93
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	38
5	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	30





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TIC Library : C:\Database\NIST20.L
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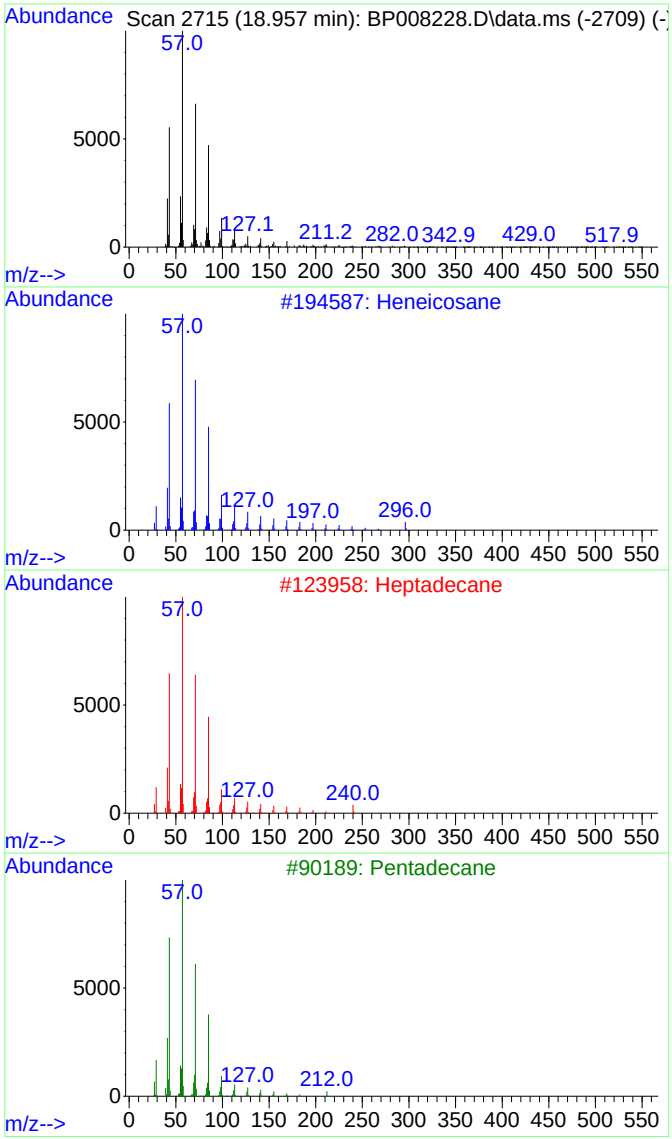
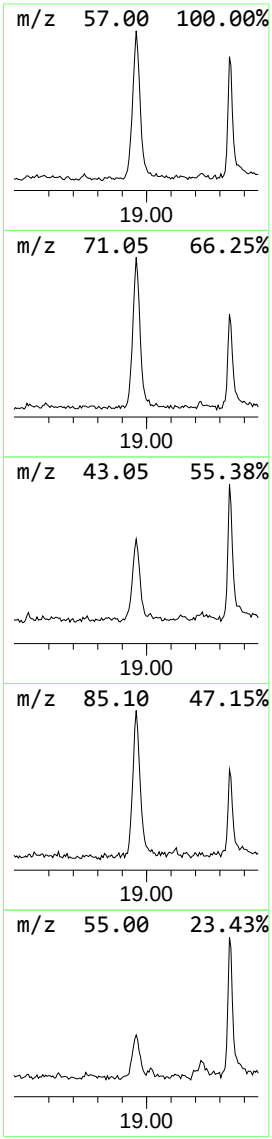
Peak Number 7 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.957	7.21 ng	309742	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane	240	C17H36	000629-78-7	95
3	Pentadecane	212	C15H32	000629-62-9	95
4	Triacontane	422	C30H62	000638-68-6	95
5	Tetracosane	338	C24H50	000646-31-1	91





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Sample : M4918-10
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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TIC Library : C:\Database\NIST20.L
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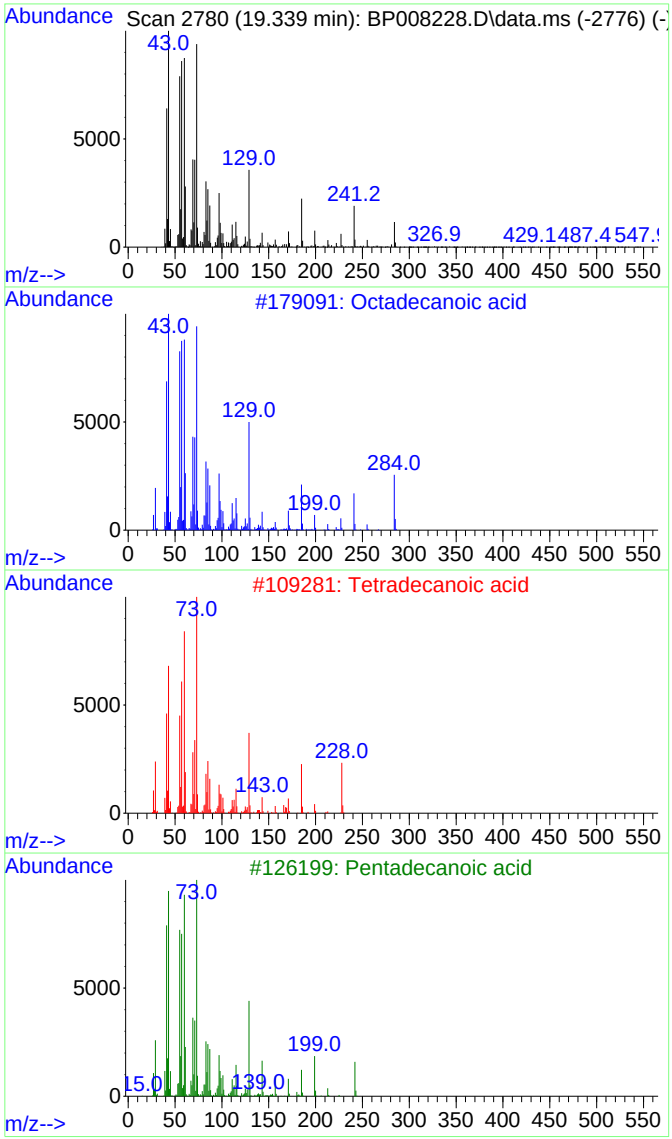
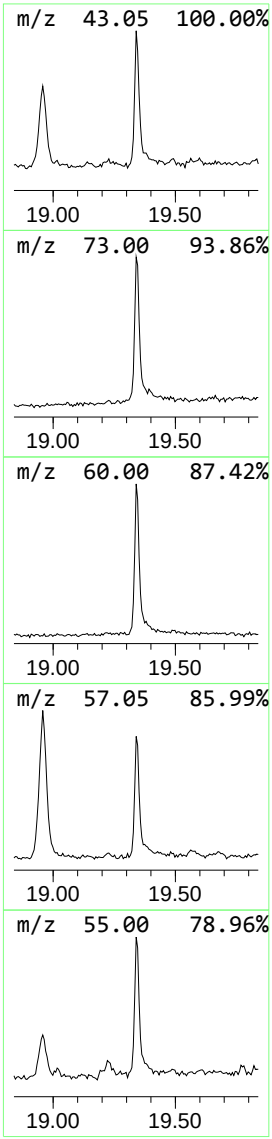
Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	9.33 ng	526560	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

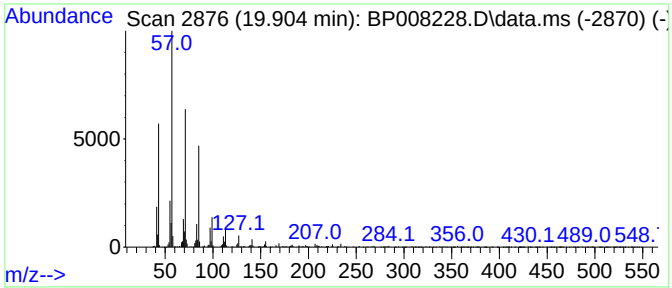
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

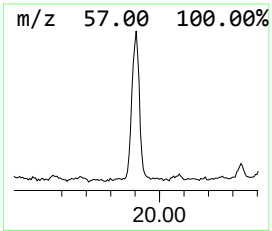
****

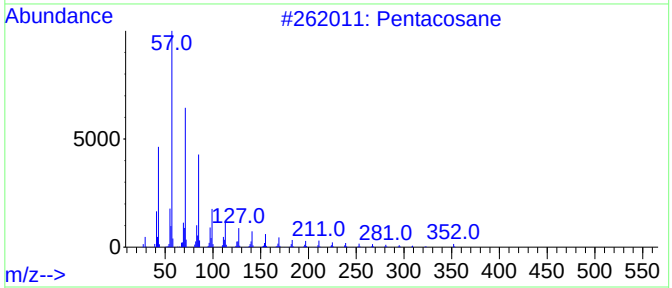
Peak Number 9 Pentacosane Concentration Rank 11

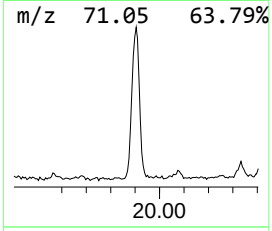
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.904	8.31 ng	468947	Chrysene-d12	21.304

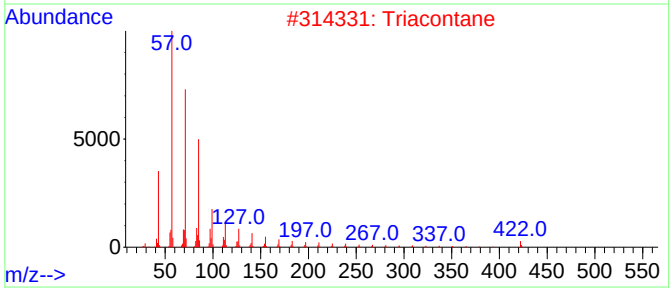
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	93
2	Triacontane	422	C30H62	000638-68-6	93
3	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90
4	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87

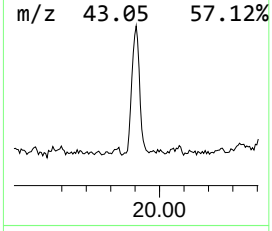


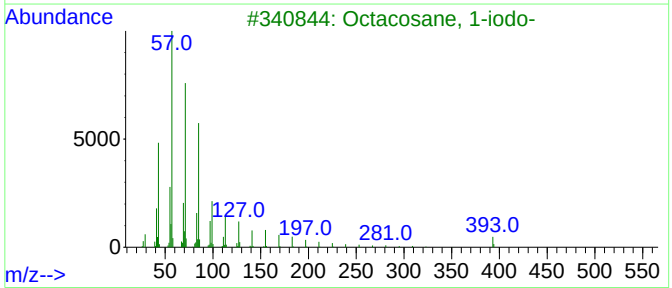


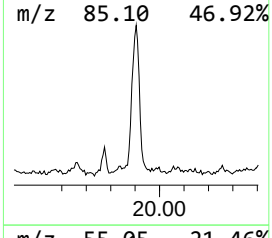


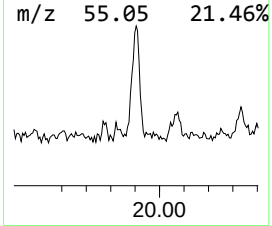












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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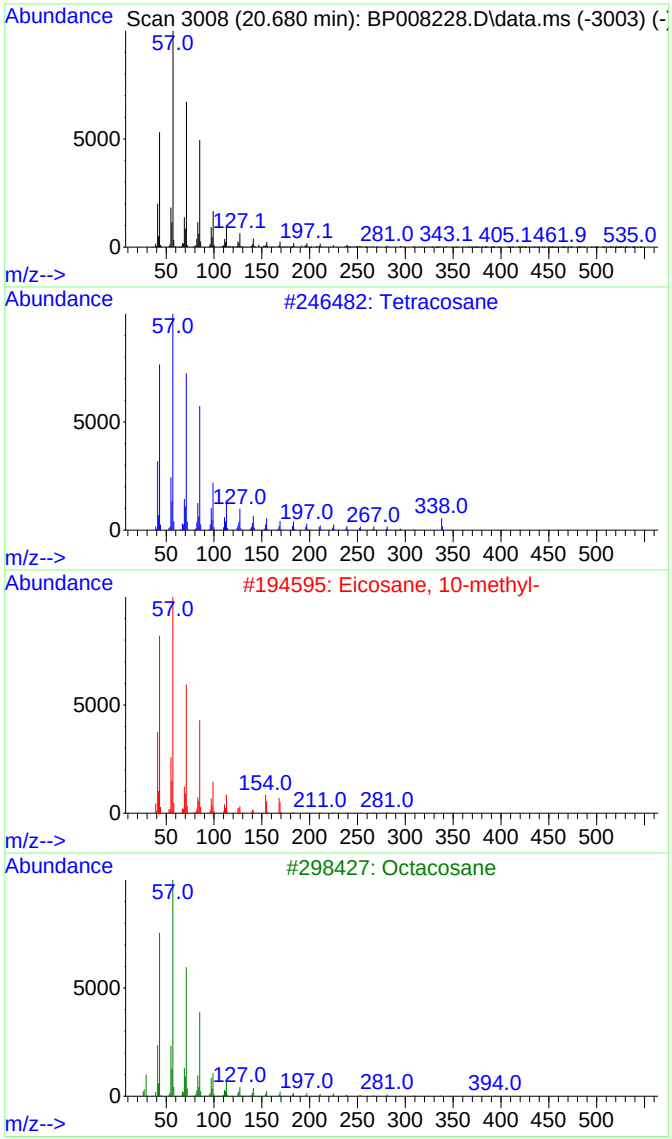
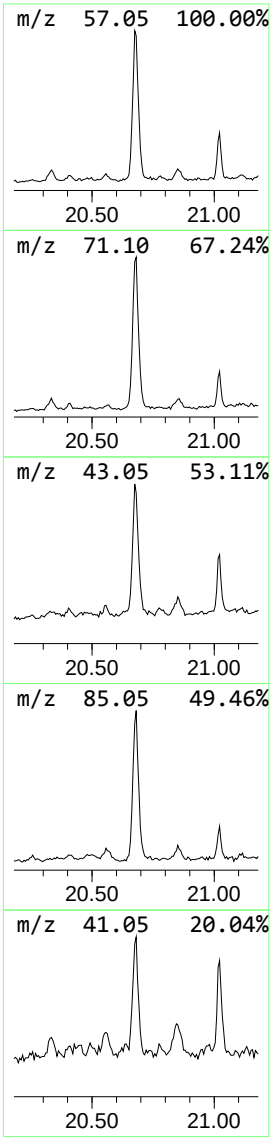
Peak Number 10 Eicosane, 10-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.680	8.65 ng	488135	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Octacosane	394	C28H58	000630-02-4	90
4	9-Methylheneicosane	310	C22H46	070475-51-3	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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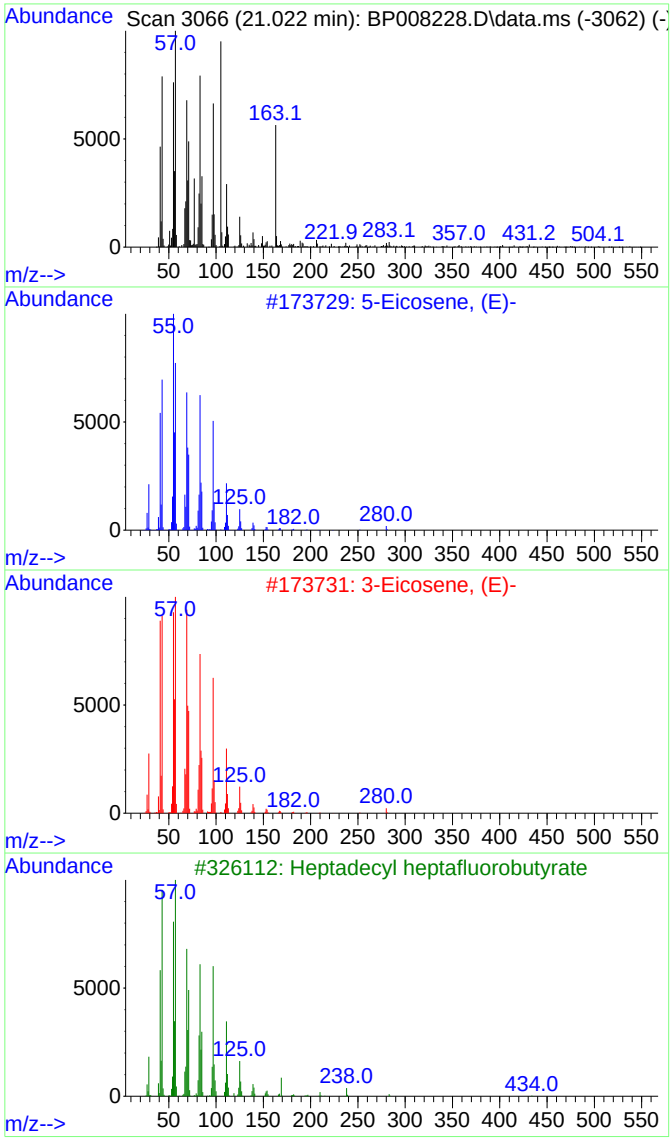
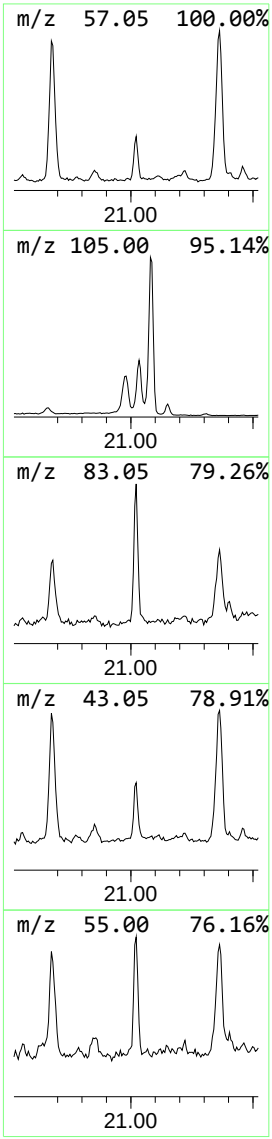
Peak Number 11 5-Eicosene, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	6.66 ng	375903	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	81
5	1-Hexacosene	364	C26H52	018835-33-1	81





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Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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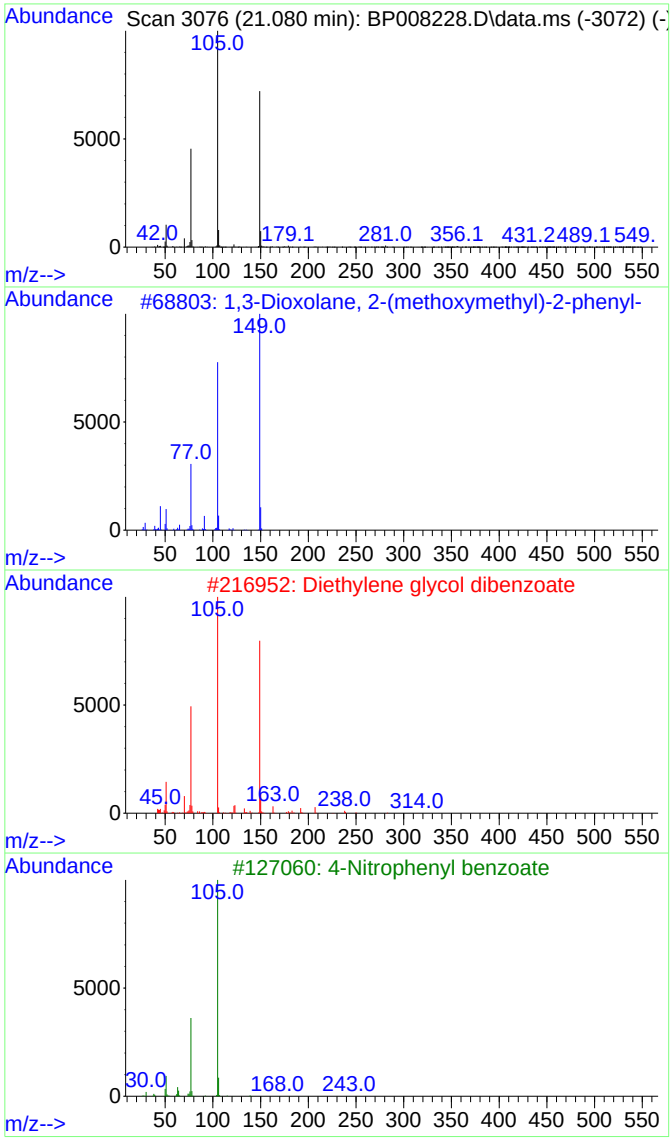
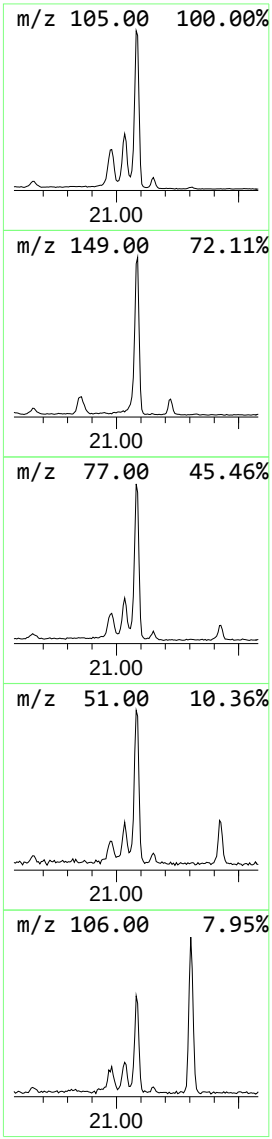
Peak Number 12 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	9.76 ng	550910	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
3	4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	49
4	2-Phenylbutenolide	160	C10H8O2	001955-39-1	49
5	Benzoic acid, 2-benzoylaminocarb...	345	C21H15NO4	1000310-96-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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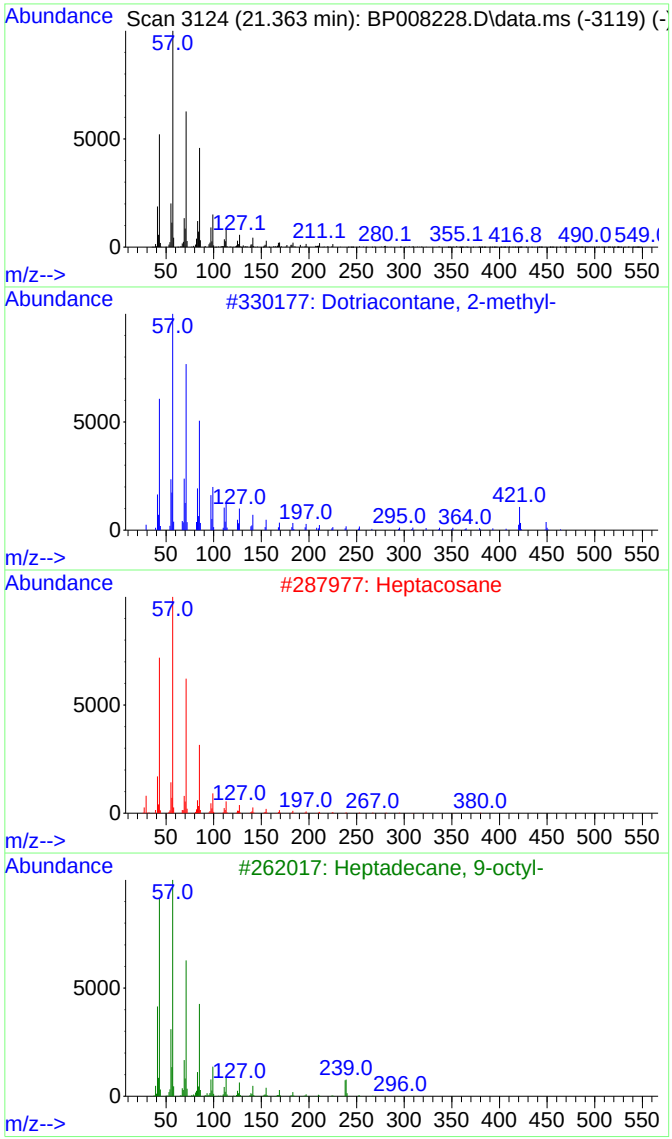
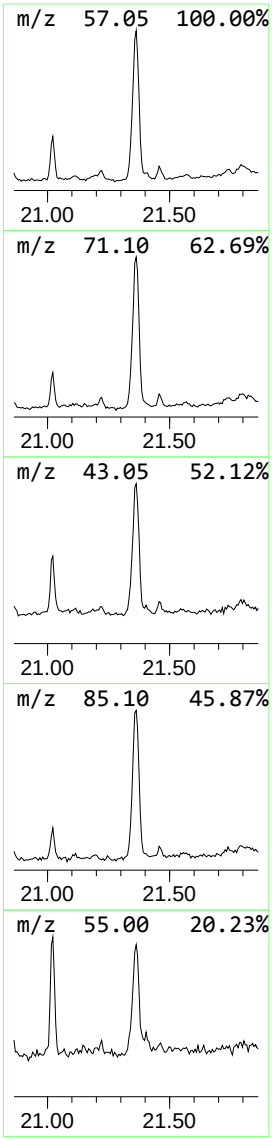
Peak Number 13 Dotriacontane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.363	10.65 ng	601087	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane, 2-methyl-	465	C33H68	001720-11-2	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90





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Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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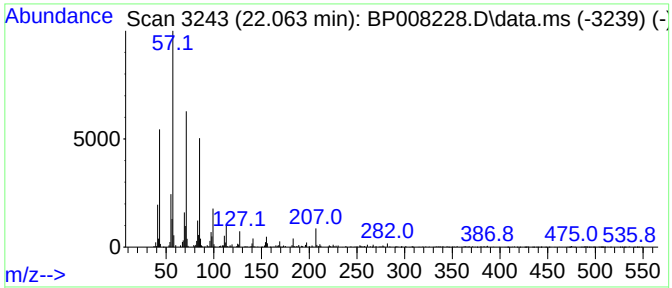
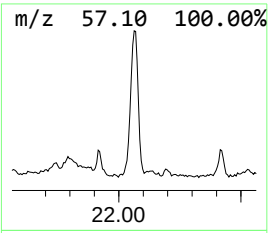
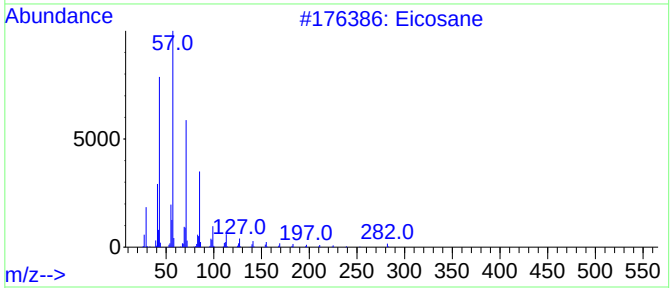
Peak Number 14 Eicosane Concentration Rank 10

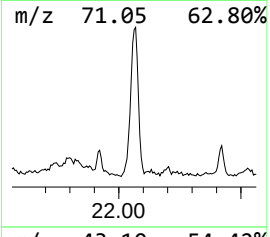
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.063	8.45 ng	476794	Chrysene-d12	21.304

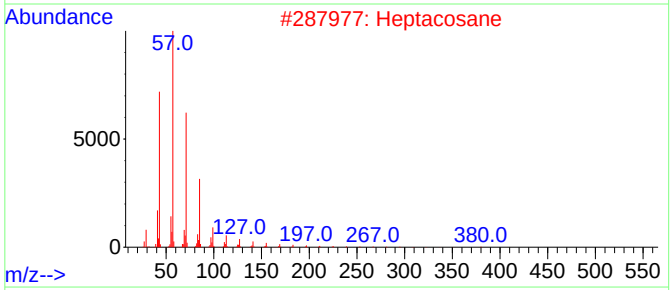
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptacosane	380	C27H56	000593-49-7	94
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90

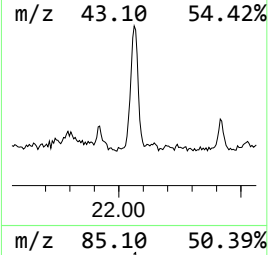


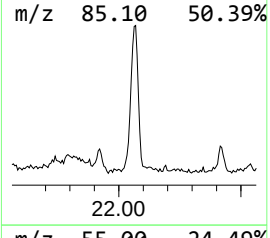


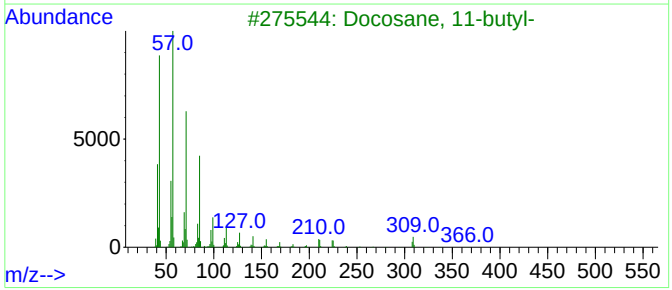


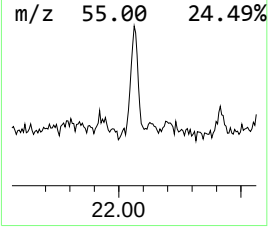












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

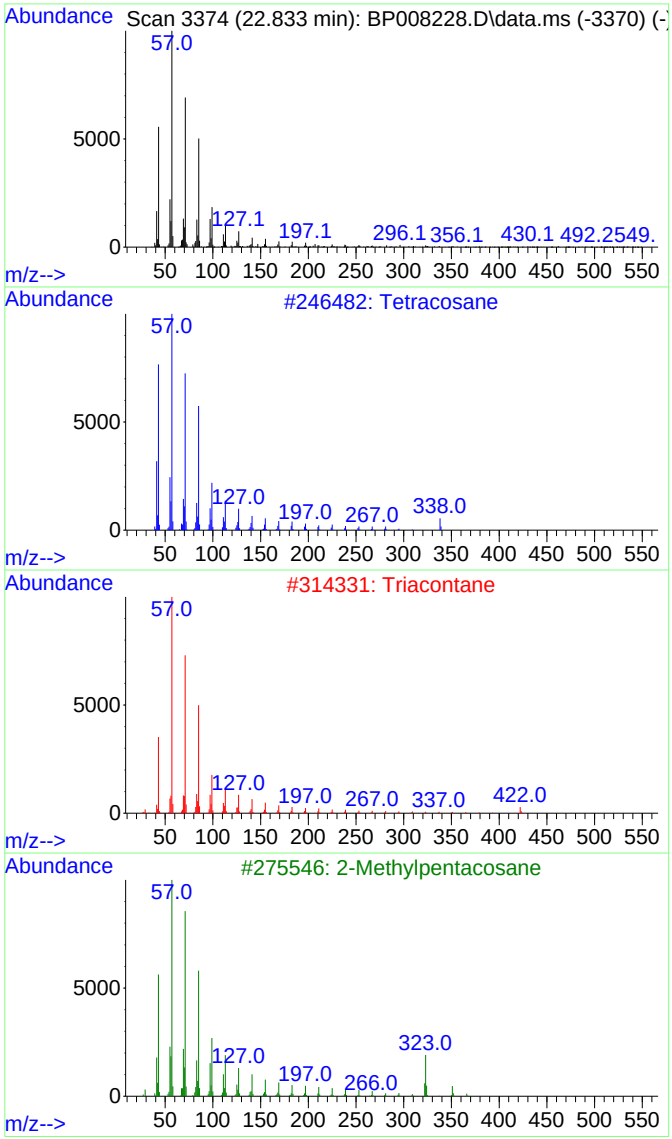
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

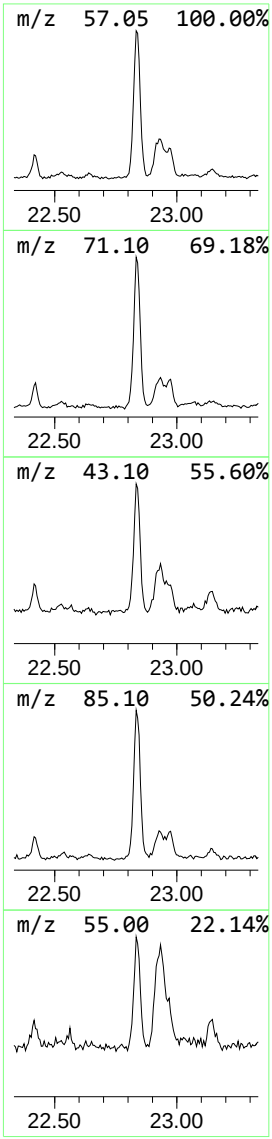
****

Peak Number 15 Tetracosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.833	5.41 ng	508279	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Triacontane	422	C30H62	000638-68-6	93
3	2-Methylpentacosane	366	C26H54	000629-87-8	93
4	Octadecane	254	C18H38	000593-45-3	91
5	Tricosane	324	C23H48	000638-67-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120621\
Data File : BP008228.D
Acq On : 06 Dec 2021 14:47
Operator : CG/JU
Sample : M4918-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-45A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
(E)-4-(3-Hydrox...	16.598	6.8	ng	292075	4	17.204	859209	20.0
Benzamide, N-pr...	17.551	169.3	ng	7272400	4	17.204	859209	20.0
Oxybis(propane-...	17.751	205.1	ng	8810950	4	17.204	859209	20.0
Diethylene glyc...	17.939	488.4	ng	20980300	4	17.204	859209	20.0
unknown18.104	18.104	52.0	ng	2234900	4	17.204	859209	20.0
trans-Sinapyl a...	18.416	14.3	ng	614490	4	17.204	859209	20.0
Heneicosane	18.957	7.2	ng	309742	4	17.204	859209	20.0
Octadecanoic acid	19.339	9.3	ng	526560	5	21.304	1128480	20.0
Pentacosane	19.904	8.3	ng	468947	5	21.304	1128480	20.0
Eicosane, 10-me...	20.680	8.7	ng	488135	5	21.304	1128480	20.0
5-Eicosene, (E)-	21.022	6.7	ng	375903	5	21.304	1128480	20.0
1,3-Dioxolane, ...	21.080	9.8	ng	550910	5	21.304	1128480	20.0
Dotriacontane, ...	21.363	10.7	ng	601087	5	21.304	1128480	20.0
Eicosane	22.063	8.4	ng	476794	5	21.304	1128480	20.0
Tetracosane	22.833	5.4	ng	508279	6	23.704	1879430	20.0