LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138545.D
Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FILL-MATERIAL-1

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_F\Methods\8270-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	20	rBV	1762982	2358879	83.83%	11.691%
2	3.398	219	223	242	rBV	57957	126087	4.48%	0.625%
3	5.092	507	511	520	rVB	150205	192030	6.82%	0.952%
4	5.492	575	579	582	rBV	2483249	2348575	83.46%	11.640%
5	6.498	745	750	753	rBV	2331701	2445277	86.90%	12.119%
6	6.863	808	812	815	rBV	654085	493737	17.55%	2.447%
7	7.428	902	908	911	rBV	1744410	1602597	56.95%	7.942%
8	7.675	947	950	954	rVB	59270	46468	1.65%	0.230%
9	8.145	1026	1030	1033	rBV	788381	651707	23.16%	3.230%
10	8.457	1079	1083	1096	rBV	90370	108728	3.86%	0.539%
11	9.222	1207	1213	1216	rBV	3369144	2813961	100.00%	13.946%
12	9.898	1324	1328	1331	rBV	934968	720450	25.60%	3.571%
13	9.992	1339	1344	1348	rBV	73583	95027	3.38%	0.471%
14	10.686	1458	1462	1465	rBV	1772851	1532390	54.46%	7.595%
15	11.380	1577	1580	1584	rBV	715921	616159	21.90%	3.054%
16	11.904	1664	1669	1678	rBV2	177556	214582	7.63%	1.063%
17	12.498	1762	1770	1780	rVB2	38845	101171	3.60%	0.501%
18	12.692	1799	1803	1810	rBV	45438	59298	2.11%	0.294%
19	12.968	1846	1850	1853	rBV	2198861	1883265	66.93%	9.333%
20	13.345	1907	1914	1921	rBV2	45879	91585	3.25%	0.454%
21	13.868	1999	2003	2016	rBV2	82099	180143	6.40%	0.893%
22	13.974	2016	2021	2025	rBV	63281	103395	3.67%	0.512%
23	14.021	2025	2029	2032	rVB	439181	414377	14.73%	2.054%
24	14.480	2104	2107	2108	rBV	43606	36716	1.30%	0.182%
25	14.504	2108	2111	2121	rVB2	79570	133180	4.73%	0.660%
26	15.004	2191	2196	2204	rBV	58704	98940	3.52%	0.490%
27	15.127	2213	2217	2221	rVB	38102	42296	1.50%	0.210%
28	15.486	2273	2278	2286	rBV	322856	406312	14.44%	2.014%
29	15.568	2286	2292	2299	rVV	40873	70582	2.51%	0.350%
30	15.945	2351	2356	2361	rBV	32432	47645	1.69%	0.236%
31	16.033	2365	2371	2374	rBV7	16740	37933	1.35%	0.188%
32	16.209	2396	2401	2410	rVB3	29413	63618	2.26%	0.315%
33	16.962	2523	2529	2536	rVB5	15528	40382	1.44%	0.200%

Sum of corrected areas: 20177492

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
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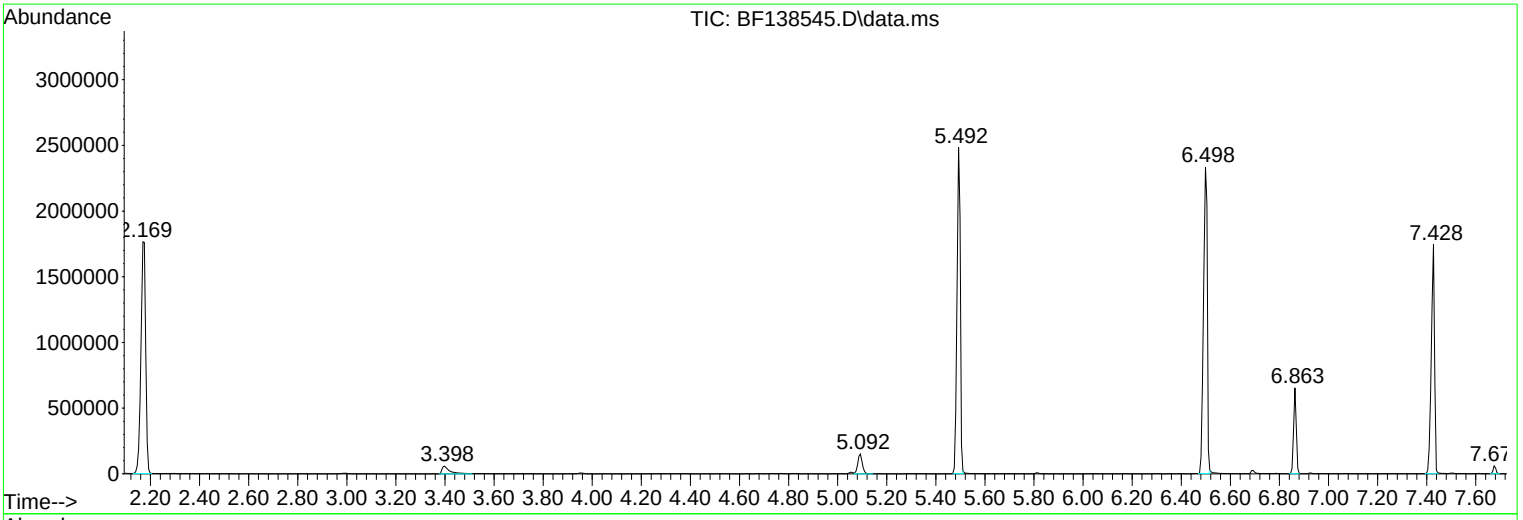
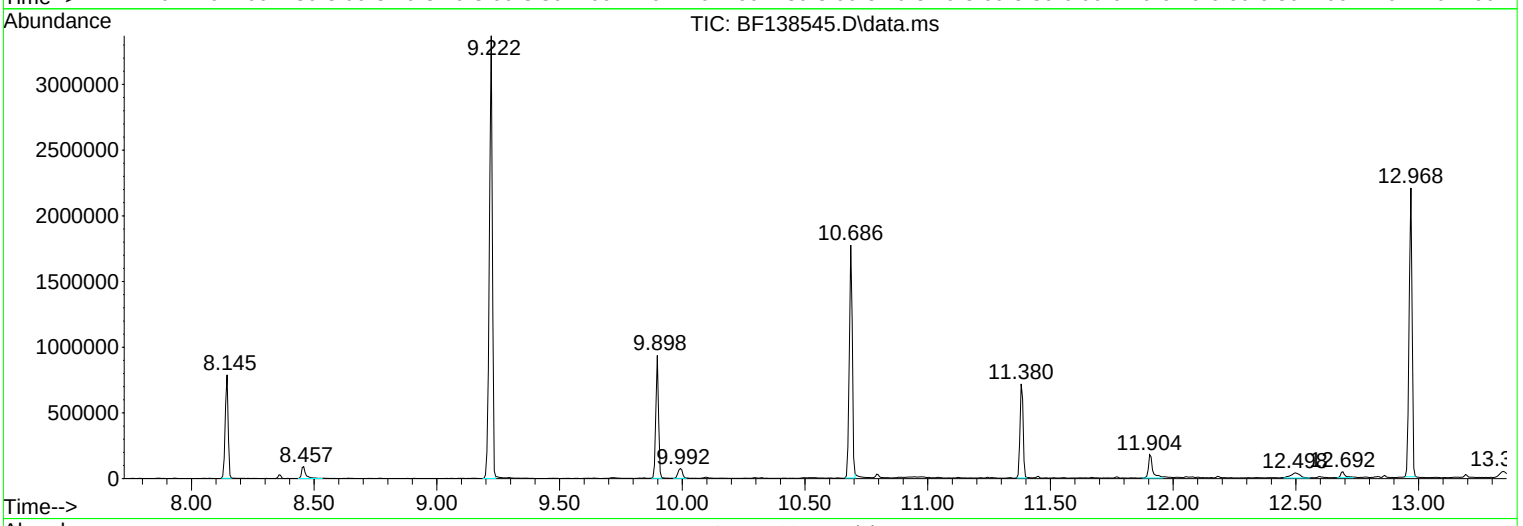
Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

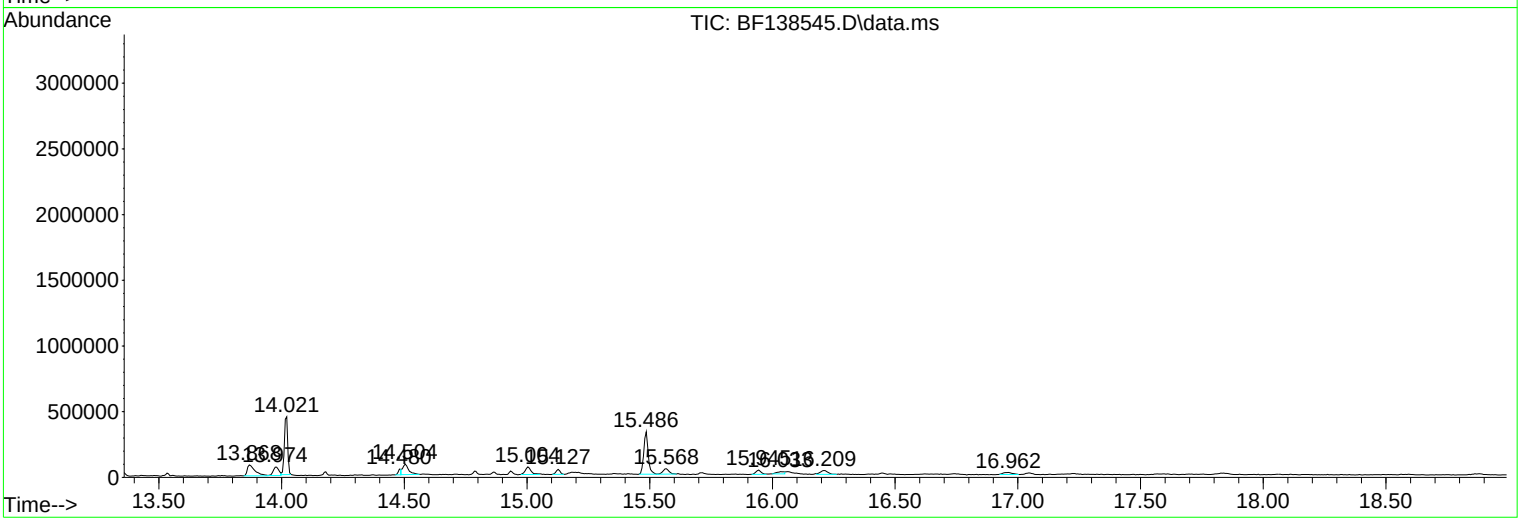
Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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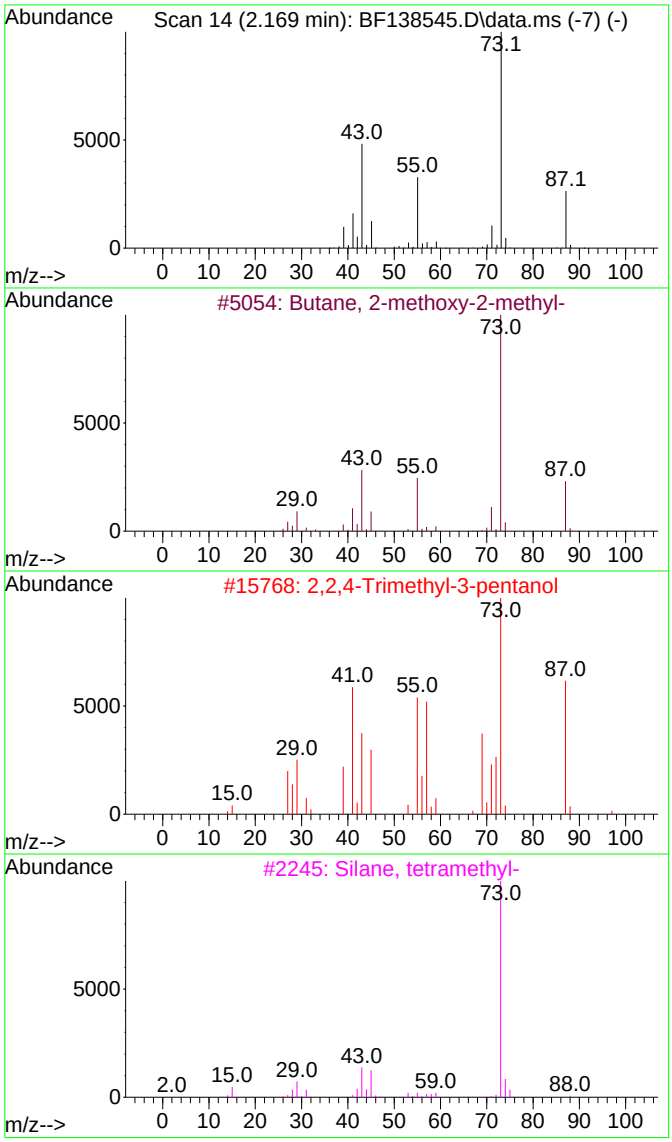
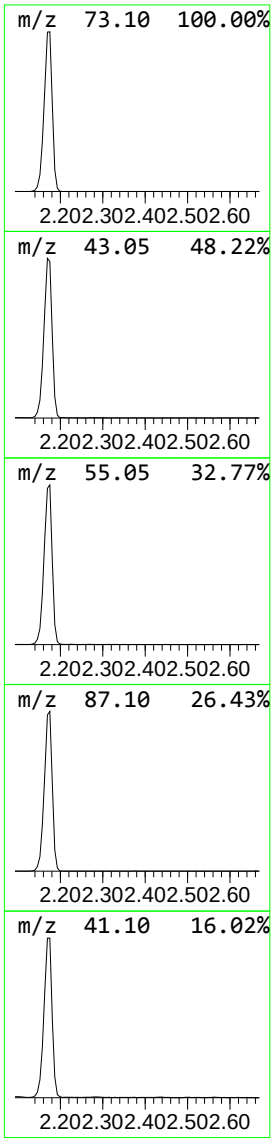
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	95.55 ng	2358880	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF138545.D
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Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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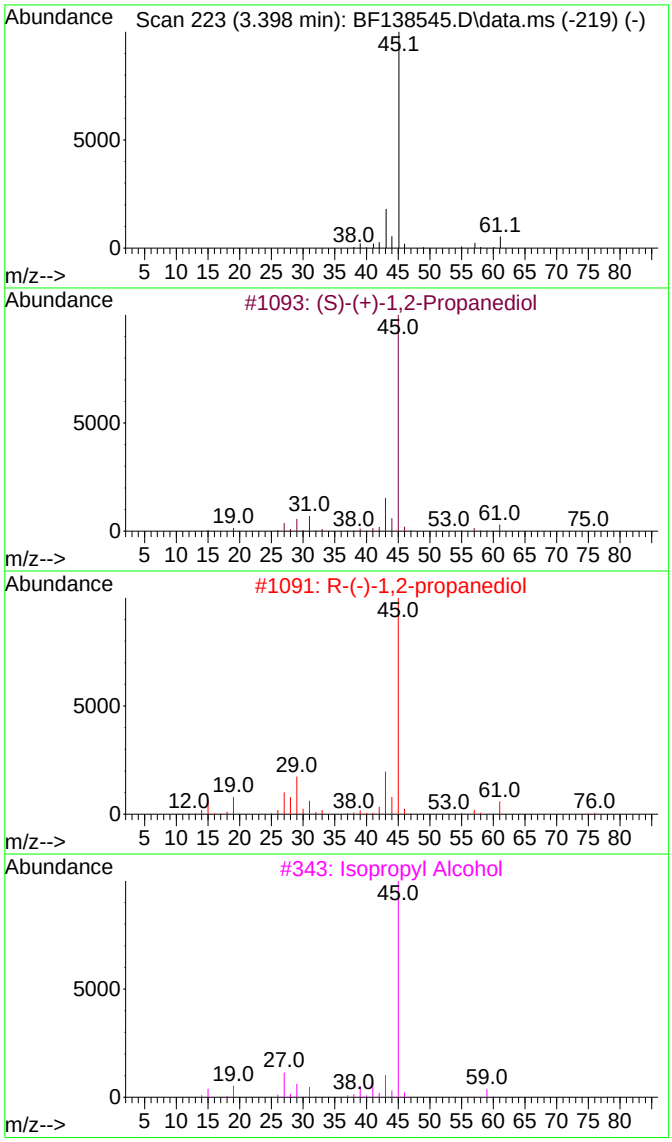
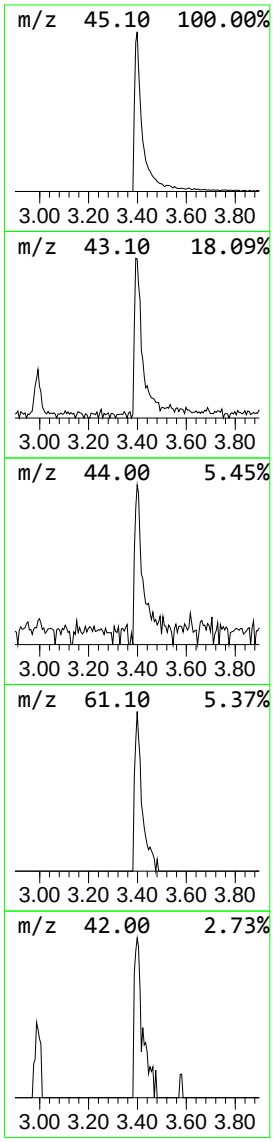
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.398	5.11 ng	126087	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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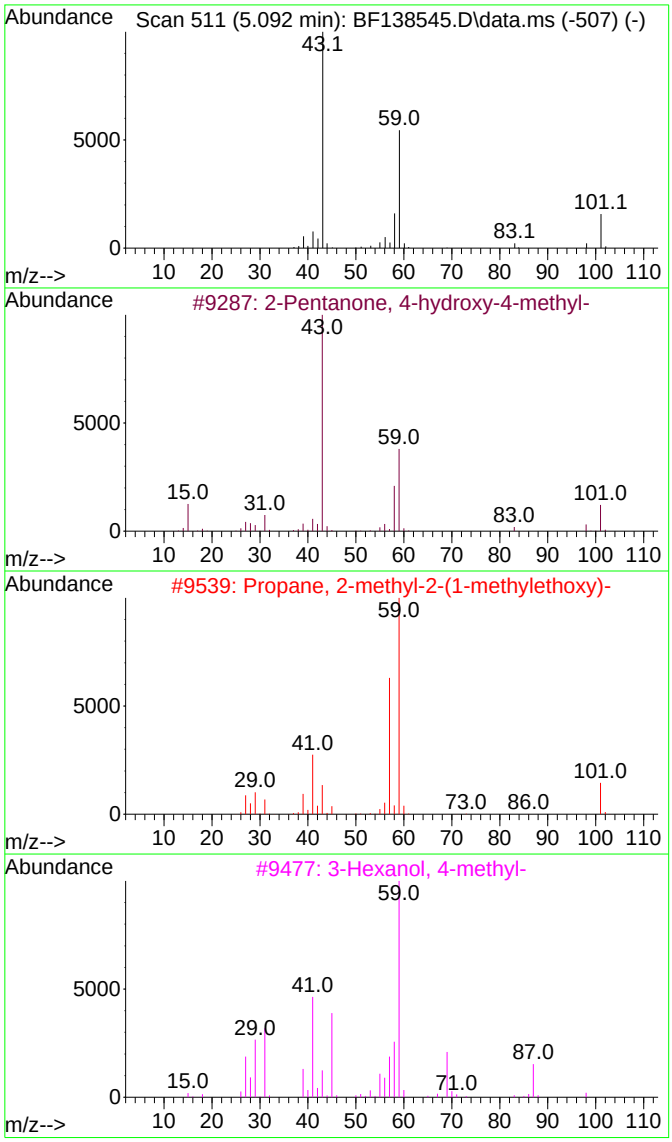
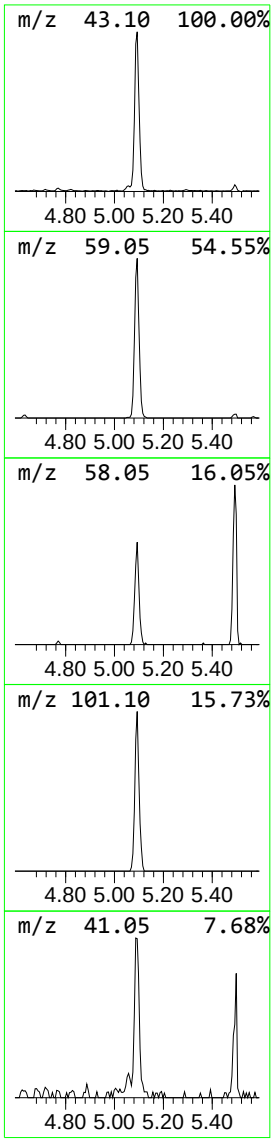
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	7.78 ng	192030	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





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Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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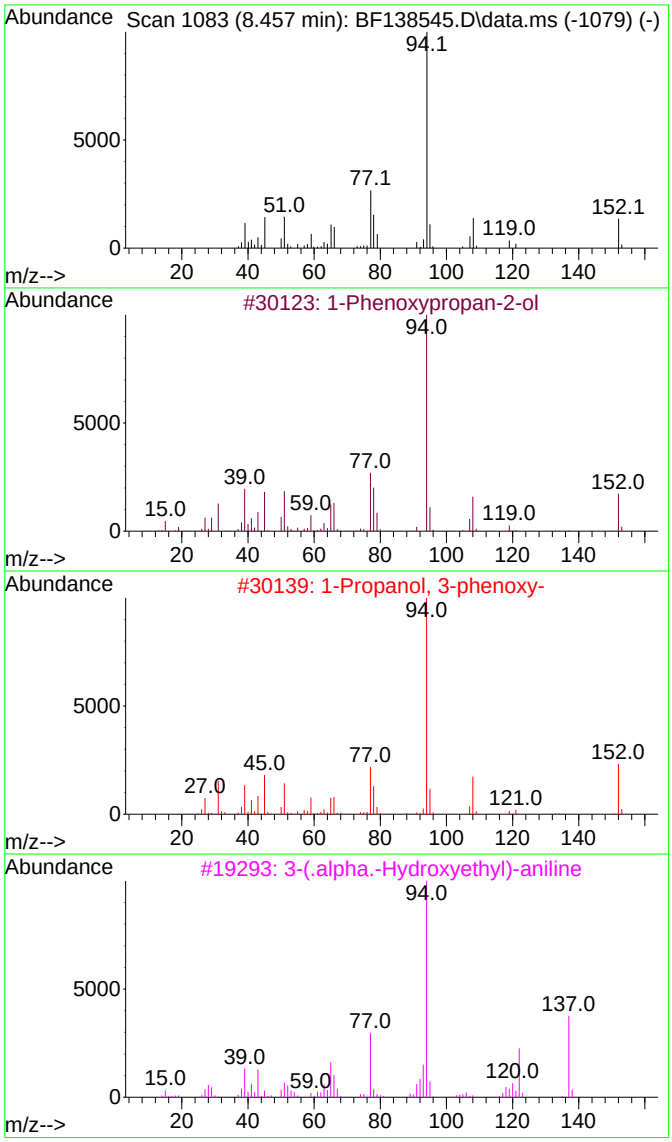
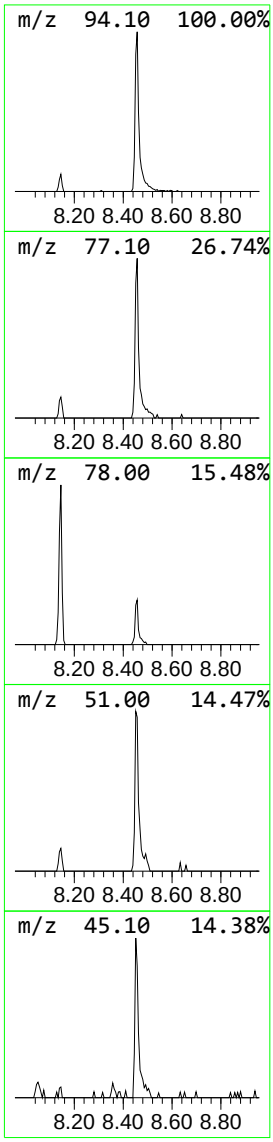
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	3.34 ng	108728	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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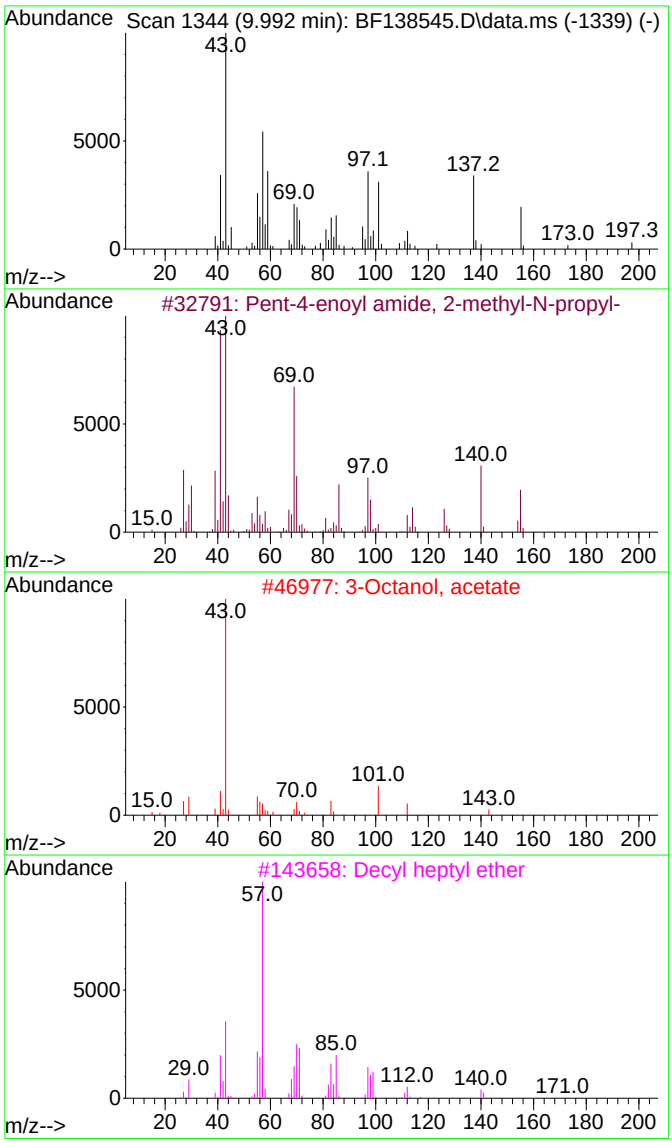
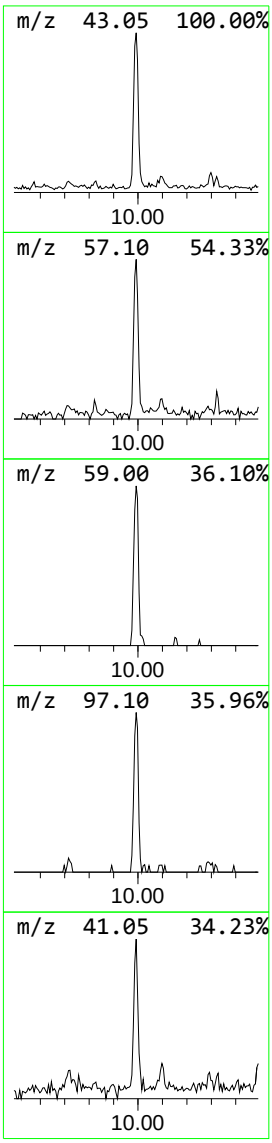
Peak Number 5 unknown9.992 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	2.64 ng	95027	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	22
2	3-Octanol, acetate	172	C10H20O2	004864-61-3	14
3	Decyl heptyl ether	256	C17H36O	1000406-39-1	11
4	1-Bromoeicosane	360	C20H41Br	004276-49-7	10
5	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
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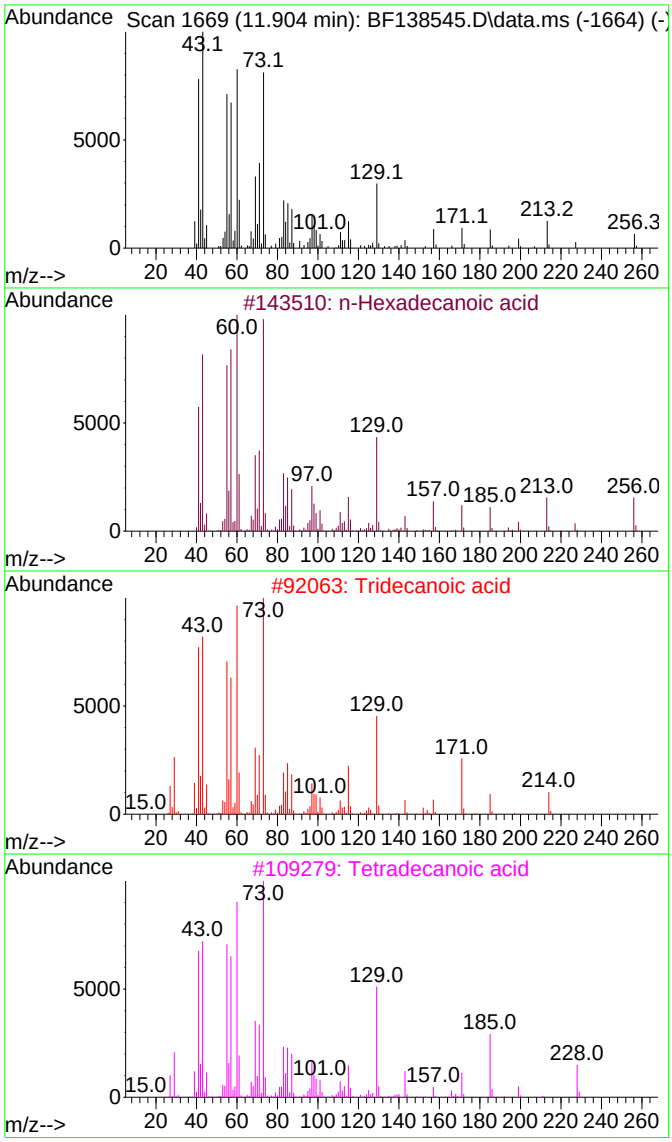
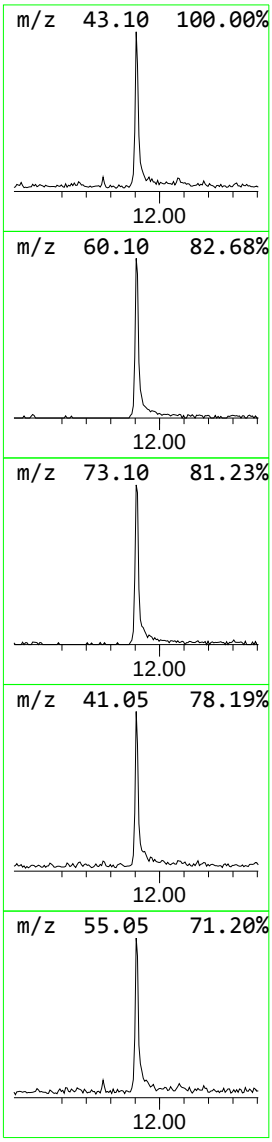
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	6.97 ng	214582	Phenanthrene-d10	11.380

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Operator : CG\JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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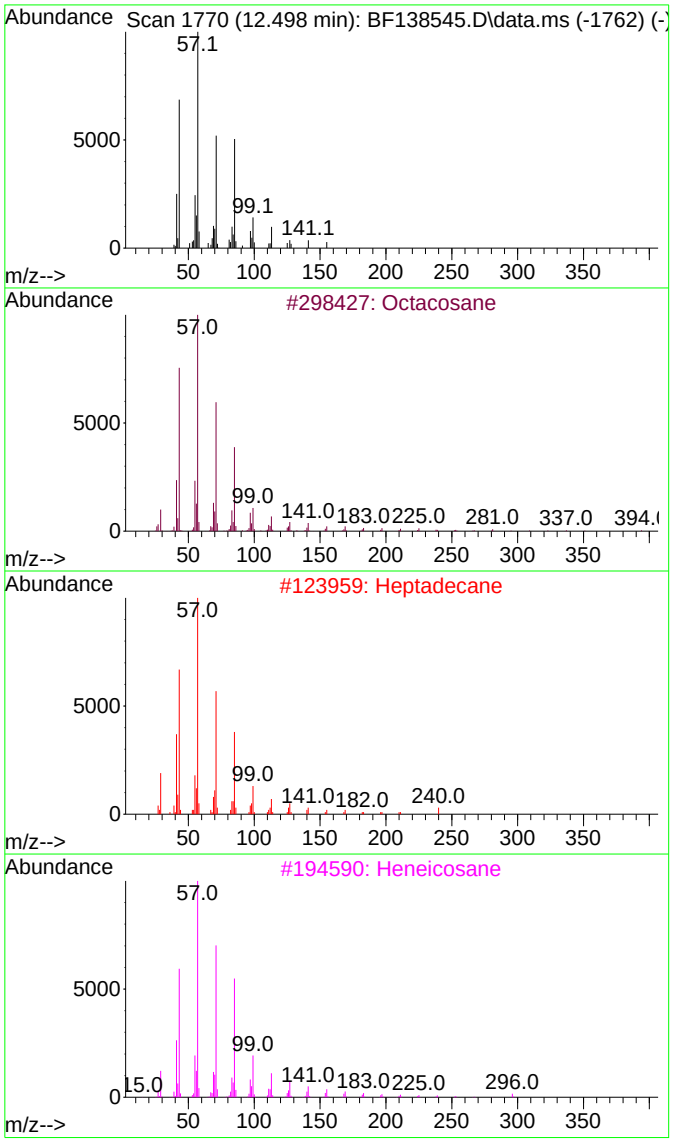
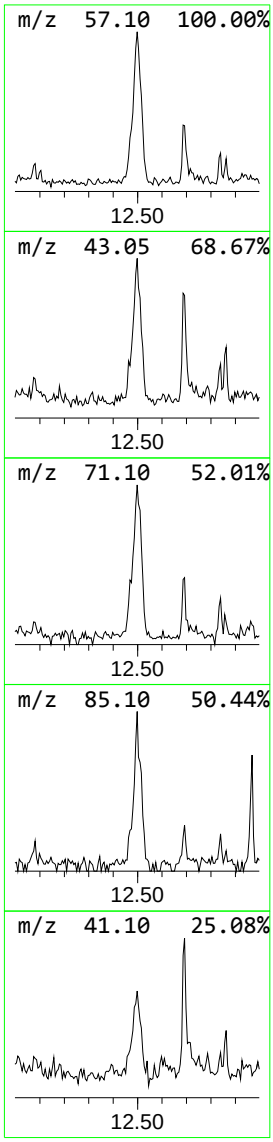
Peak Number 7 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	3.28 ng	101171	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptadecane	240	C17H36	000629-78-7	80
3	Heneicosane	296	C21H44	000629-94-7	74
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Heptacosane	380	C27H56	000593-49-7	72





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Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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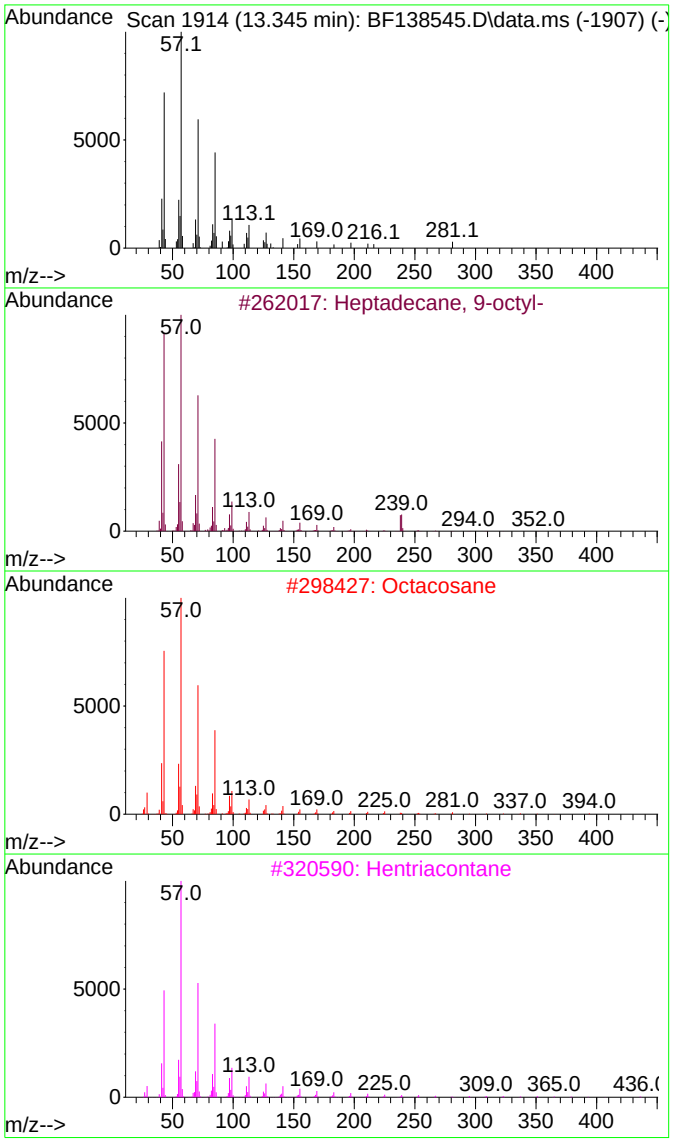
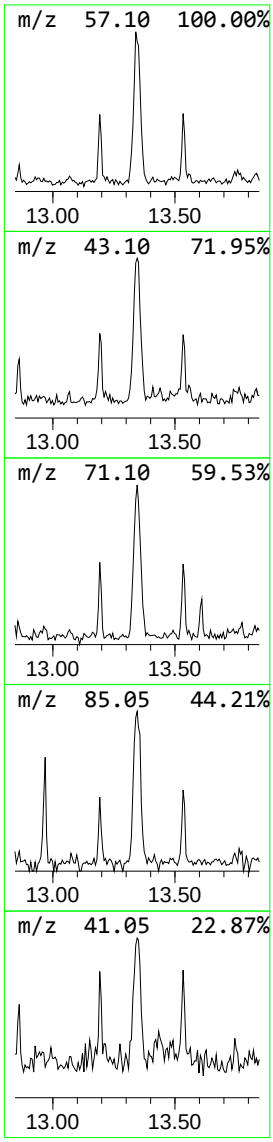
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.345	4.42 ng	91585	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Eicosane	282	C20H42	000112-95-8	91





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Data File : BF138545.D
Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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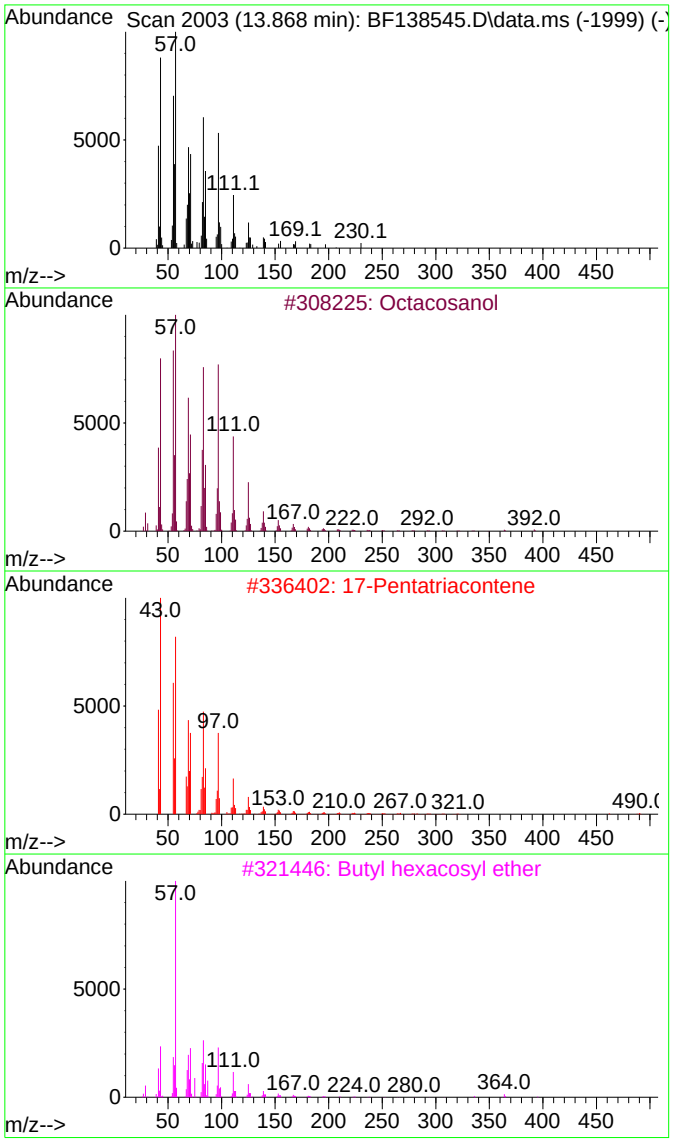
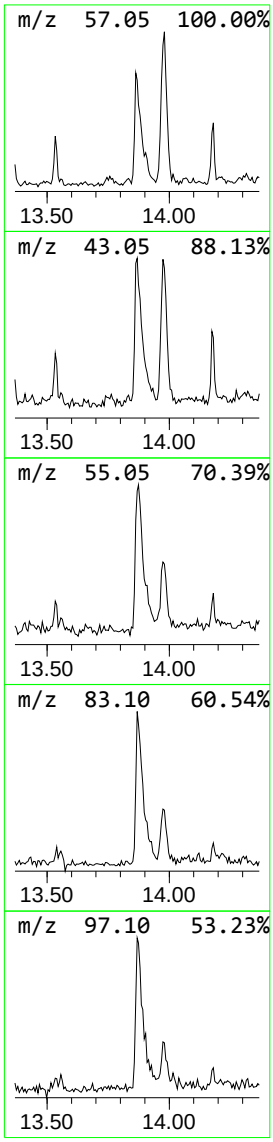
Peak Number 9 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	8.69 ng	180143	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Butyl hexacosyl ether	438	C30H62O	1000406-41-0	87
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
5	Butyl docosyl ether	382	C26H54O	1000406-40-8	87





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Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

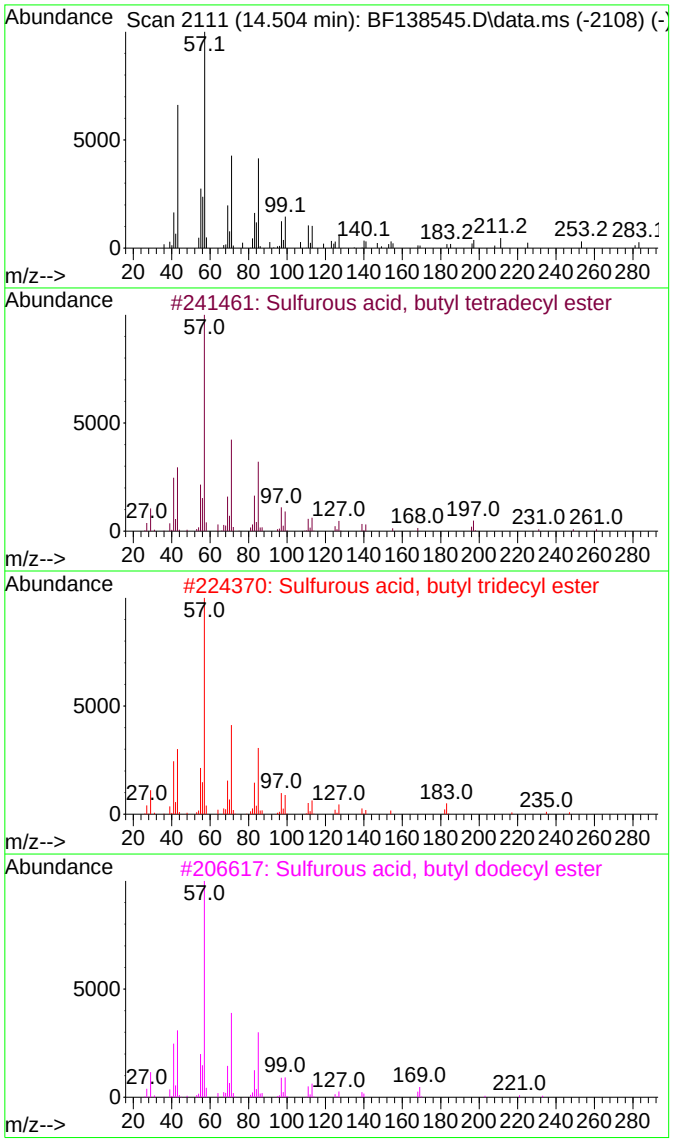
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

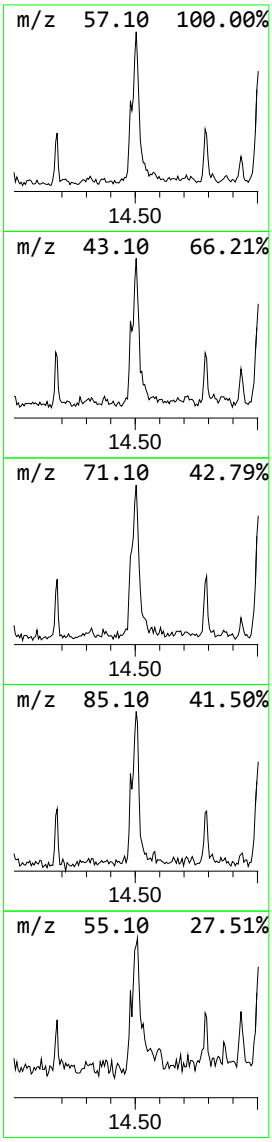
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Sulfurous acid, butyl tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	6.43 ng	133180	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	87
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	87
3	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
5	2-Methyltetracosane	352	C25H52	001560-78-7	72





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Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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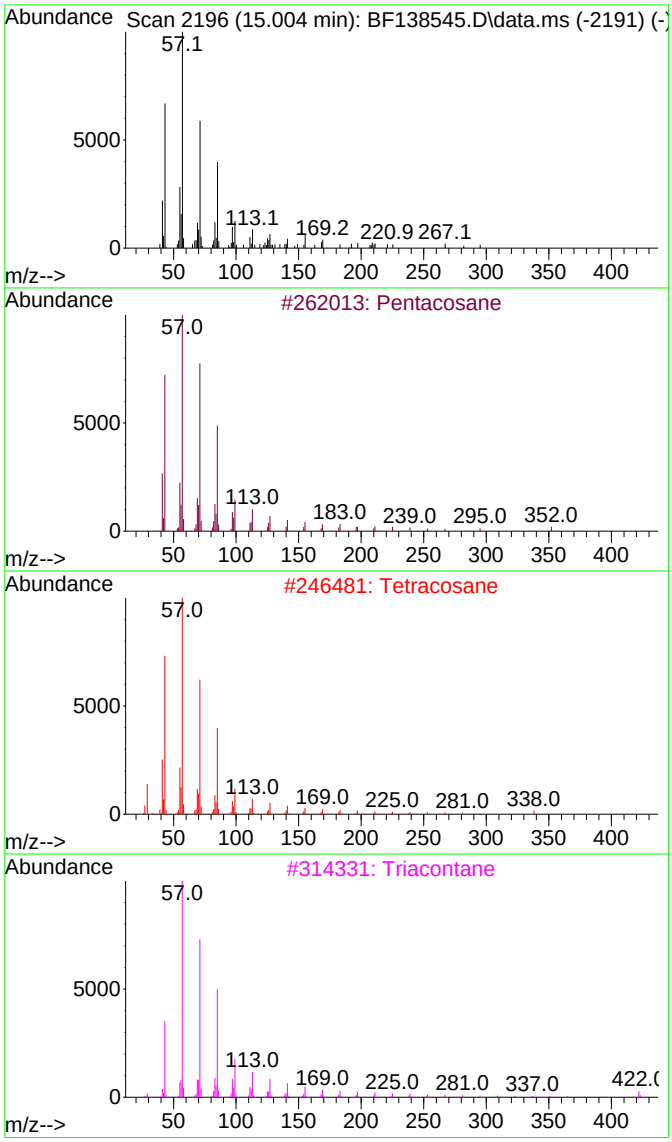
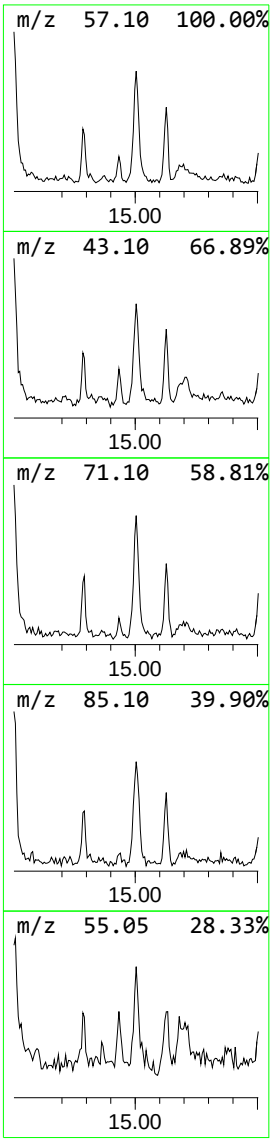
Peak Number 11 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	4.87 ng	98940	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Hentriacontane	437	C31H64	000630-04-6	90





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Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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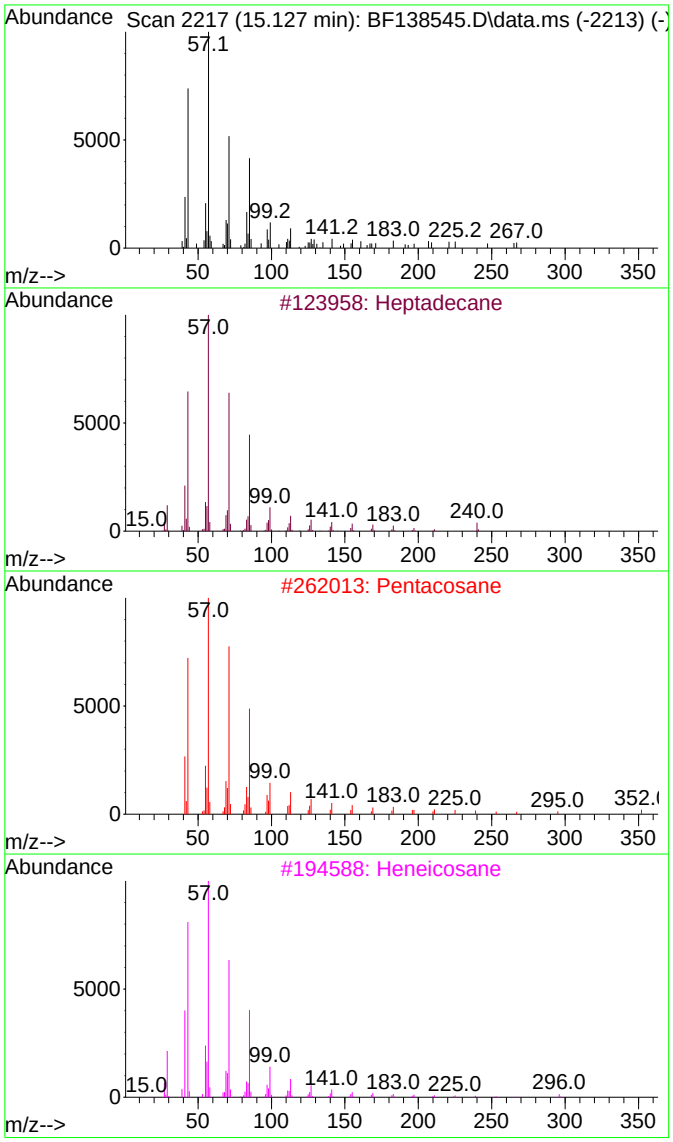
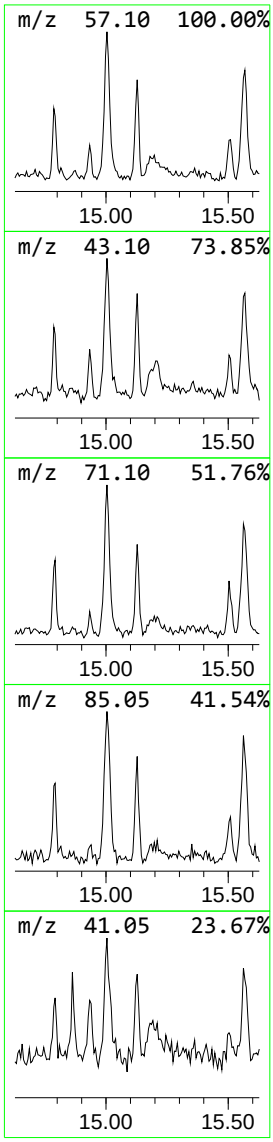
Peak Number 12 Heptadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.08 ng	42296	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Pentacosane	352	C25H52	000629-99-2	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
5	Tetratetracontane	619	C44H90	007098-22-8	86





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Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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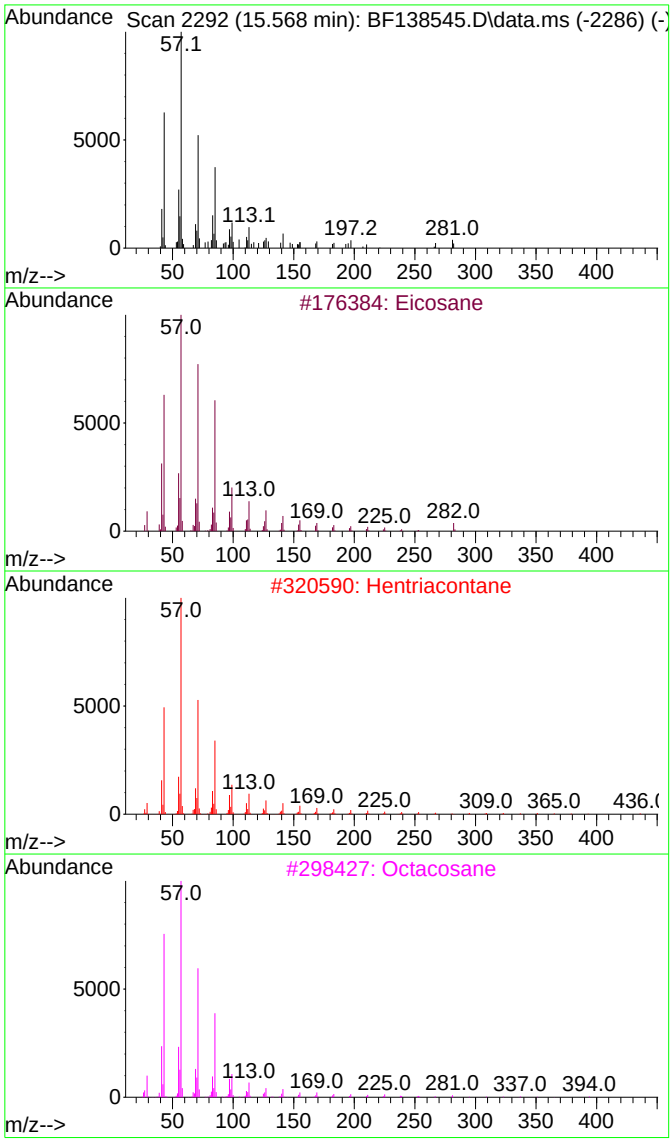
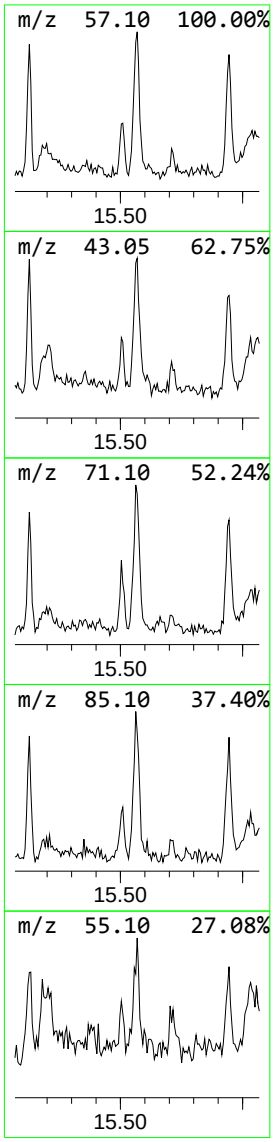
Peak Number 13 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.568	3.47 ng	70582	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Octadecane	254	C18H38	000593-45-3	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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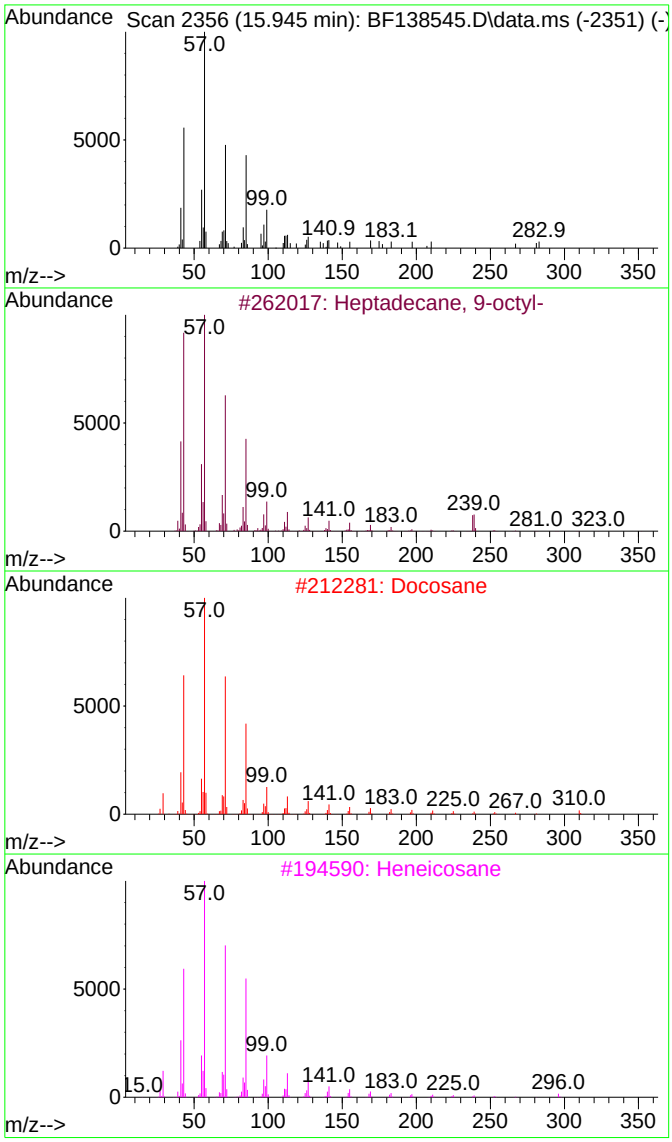
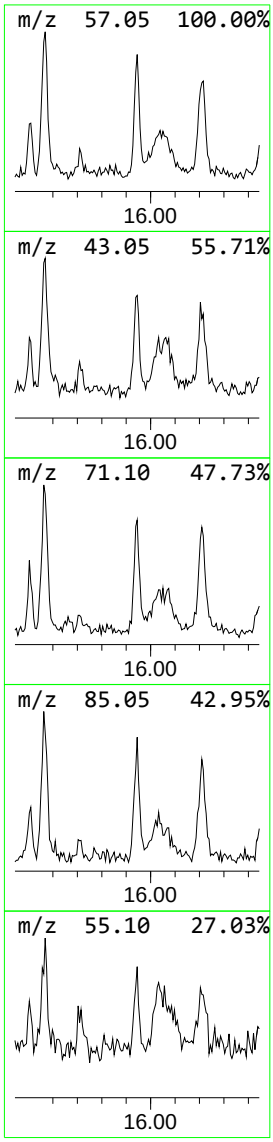
Peak Number 14 Docosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.35 ng	47645	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2	Docosane	310	C22H46	000629-97-0	86
3	Heneicosane	296	C21H44	000629-94-7	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138545.D
Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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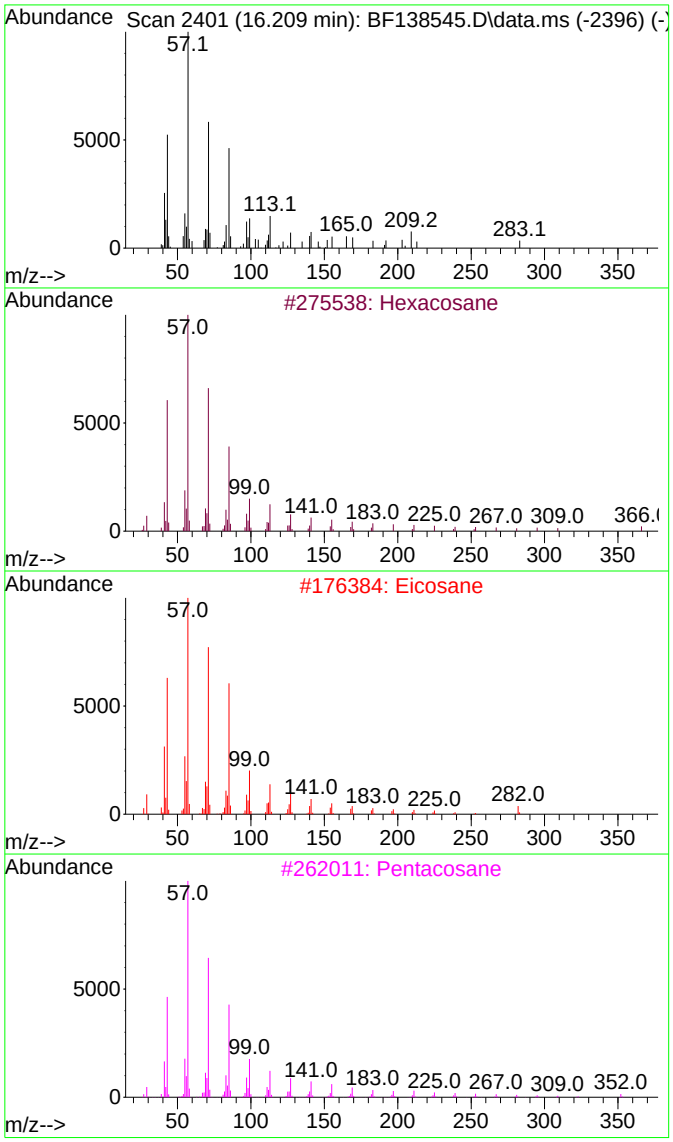
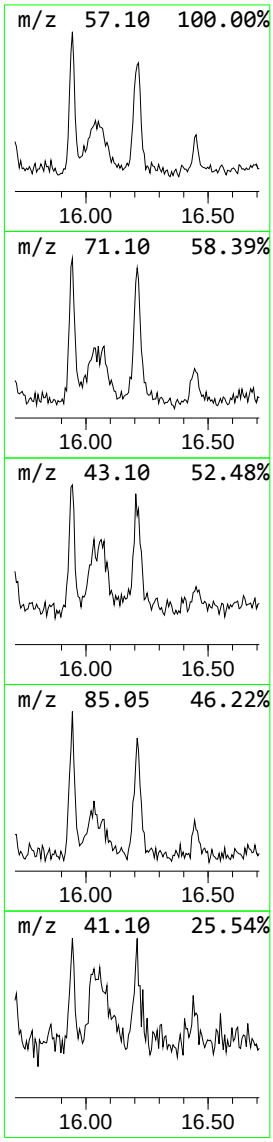
Peak Number 15 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	3.13 ng	63618	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Eicosane	282	C20H42	000112-95-8	83
3	Pentacosane	352	C25H52	000629-99-2	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138545.D
Acq On : 12 Jul 2024 14:33
Operator : CG\JU
Sample : P3193-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.169	95.5	ng	2358880	1	6.863	493737	20.0
(S)-(+)-1,2-Pro...	3.398	5.1	ng	126087	1	6.863	493737	20.0
2-Pentanone, 4-...	5.092	7.8	ng	192030	1	6.863	493737	20.0
1-Phenoxypropan...	8.457	3.3	ng	108728	2	8.145	651707	20.0
unknown9.992	9.992	2.6	ng	95027	3	9.898	720450	20.0
n-Hexadecanoic ...	11.904	7.0	ng	214582	4	11.380	616159	20.0
Octacosane	12.498	3.3	ng	101171	4	11.380	616159	20.0
Heptadecane, 9-...	13.345	4.4	ng	91585	5	14.021	414377	20.0
Octacosanol	13.868	8.7	ng	180143	5	14.021	414377	20.0
Sulfurous acid,...	14.504	6.4	ng	133180	5	14.021	414377	20.0
Pentacosane	15.004	4.9	ng	98940	6	15.486	406312	20.0
Heptadecane	15.127	2.1	ng	42296	6	15.486	406312	20.0
Eicosane	15.568	3.5	ng	70582	6	15.486	406312	20.0
Docosane	15.945	2.4	ng	47645	6	15.486	406312	20.0
Hexacosane	16.209	3.1	ng	63618	6	15.486	406312	20.0