LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211058-SI-COMP-3-MODIFIED-EL

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	31	rVB	2531871	3418293	88.94%	12.257%
2	5.516	579	583	593	rBV	1887921	1857996	48.34%	6.662%
3	6.522	750	754	763	rBV	1401476	1278592	33.27%	4.585%
4	6.898	814	818	821	rBV	995285	797412	20.75%	2.859%
5	7.463	907	914	917	rBV	2268550	2330893	60.65%	8.358%
6	7.545	924	928	941	rVB2	49814	72119	1.88%	0.259%
7	8.098	1018	1022	1030	rBV5	25197	60686	1.58%	0.218%
8	8.181	1032	1036	1044	rVV	1185521	995450	25.90%	3.569%
9	9.257	1214	1219	1222	rBV	4320372	3843257	100.00%	13.781%
10	9.645	1282	1285	1288	rBV	263994	212162	5.52%	0.761%
11	9.933	1327	1334	1338	rBV	1206448	1111210	28.91%	3.985%
12	10.128	1364	1367	1374	rBV6	27173	45092	1.17%	0.162%
13	10.345	1400	1404	1409	rVB2	33049	43540	1.13%	0.156%
14	10.728	1464	1469	1472	rBV	2548254	2340693	60.90%	8.393%
15	11.422	1583	1587	1594	rBV	1135835	981174	25.53%	3.518%
16	11.580	1611	1614	1618	rBV	889637	706153	18.37%	2.532%
17	11.804	1648	1652	1655	rVB2	134230	112065	2.92%	0.402%
18	11.939	1670	1675	1680	rBV	536662	638156	16.60%	2.288%
19	12.092	1698	1701	1706	rVB5	29127	42209	1.10%	0.151%
20	12.492	1758	1769	1779	rBV2	59204	179767	4.68%	0.645%
21	12.633	1790	1793	1799	rBV7	27740	48999	1.27%	0.176%
22	12.727	1802	1809	1818	rVV2	276186	359169	9.35%	1.288%
23	13.010	1852	1857	1860	rBV	3505800	3126345	81.35%	11.210%
24	13.433	1921	1929	1942	rBV2	83927	237506	6.18%	0.852%
25	13.851	1996	2000	2003	rBV	52544	71191	1.85%	0.255%
26	13.892	2003	2007	2010	rBV2	80658	96872	2.52%	0.347%
27	13.927	2010	2013	2016	rBV	221612	208383	5.42%	0.747%
28	14.063	2033	2036	2040	rBV	821780	722050	18.79%	2.589%
29	14.110	2040	2044	2051	rVB	112878	181548	4.72%	0.651%
30	14.521	2111	2114	2116	rVB	44888	41350	1.08%	0.148%
31	14.657	2132	2137	2144	rBV	111036	197896	5.15%	0.710%
32	14.721	2144	2148	2155	rVV8	37095	59132	1.54%	0.212%
33	14.827	2161	2166	2170	rBV3	61764	117411	3.05%	0.421%
34	14.910	2178	2180	2186	rVB2	40753	44201	1.15%	0.158%
35	15.180	2223	2226	2230	rVB	38218	41563	1.08%	0.149%
36	15.233	2230	2235	2244	rVB	83570	154030	4.01%	0.552%

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.557	2285	2290	2299	rBV	643414	835937	21.75%	2.998%
38	15.904	2344	2349	2356	rVB	62481	125595	3.27%	0.450%
39	16.657	2474	2477	2485	rVB3	42678	78397	2.04%	0.281%
40	17.074	2544	2548	2556	rVB4	36470	73214	1.90%	0.263%

Sum of corrected areas: 27887708

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
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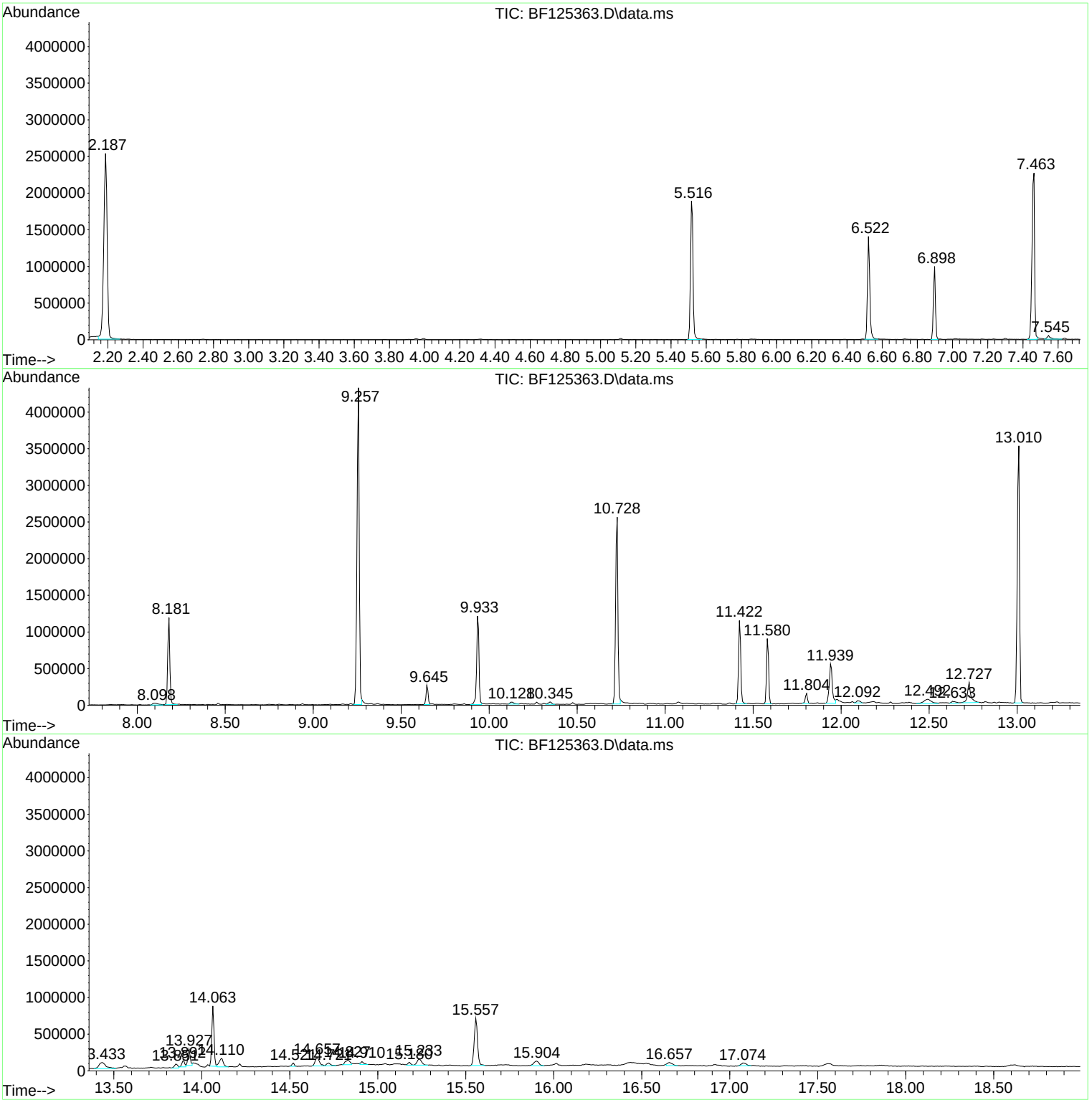
Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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_F\Data\BF090421\
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Operator : JU/CG
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Instrument :
BNA_F
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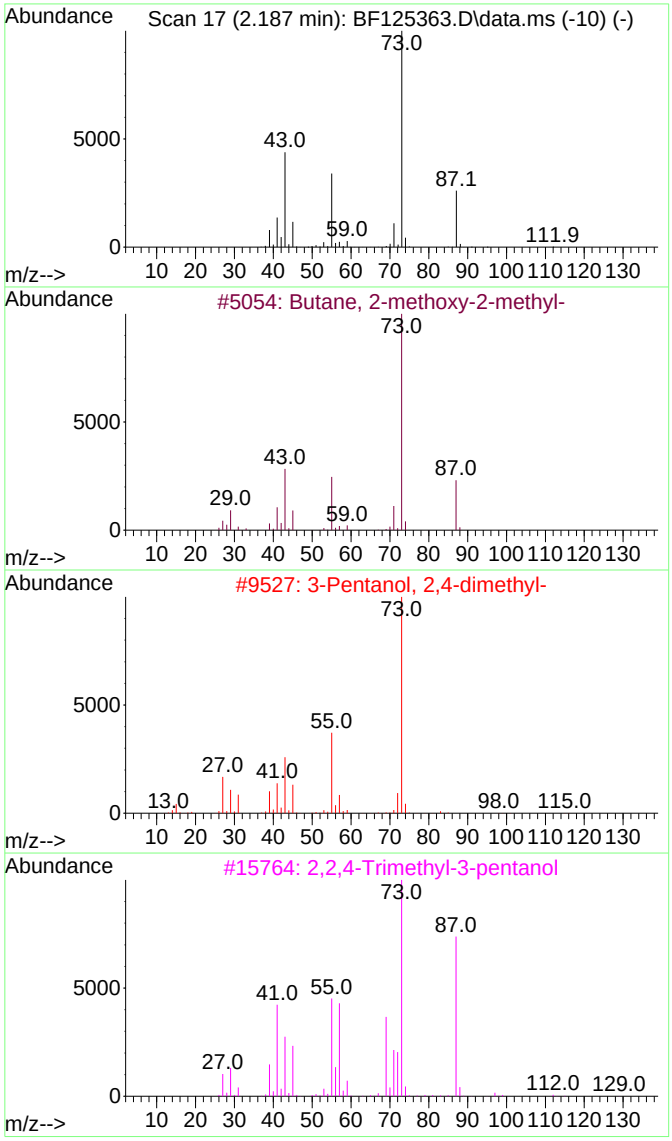
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

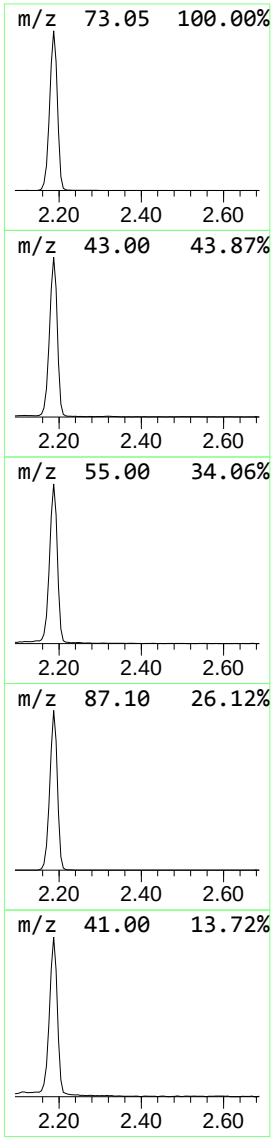
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	85.73 ng	3418290	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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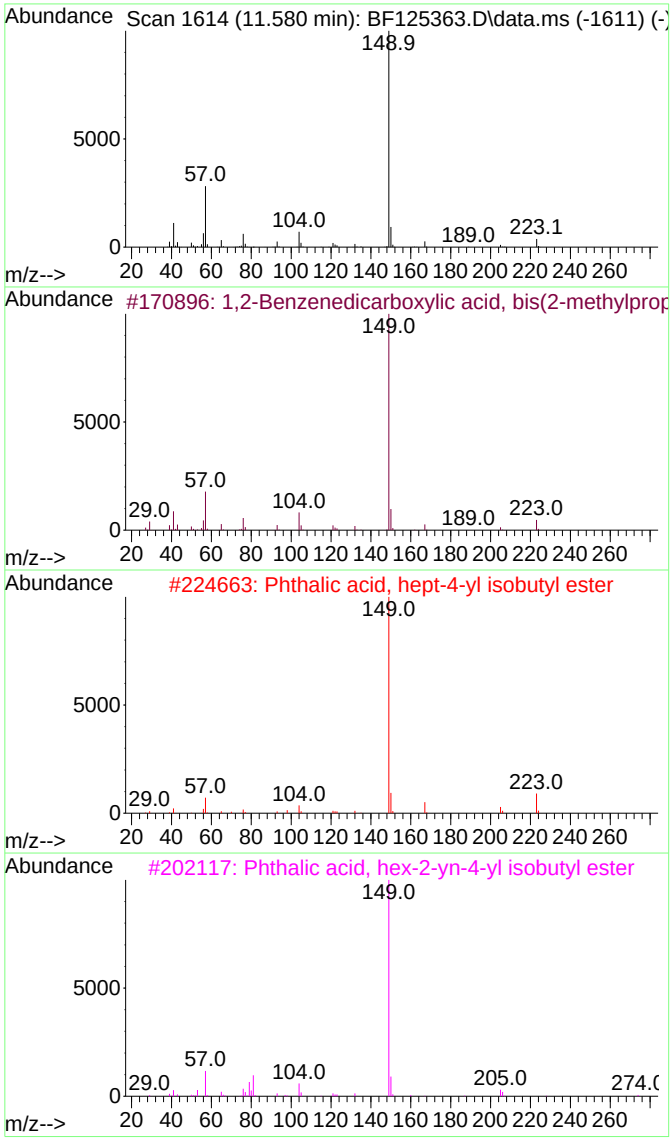
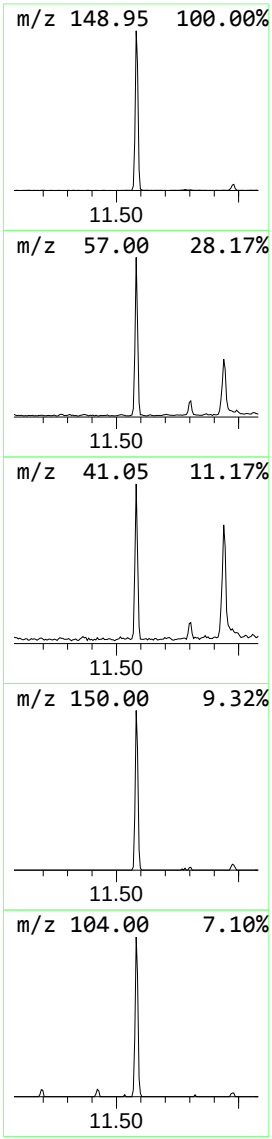
****
Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	14.39 ng	706153	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2	Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	83
3	Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78
4	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	78
5	Phthalic acid, 6-ethyl-3-octyl i...	362	C22H34O4	1000315-17-9	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

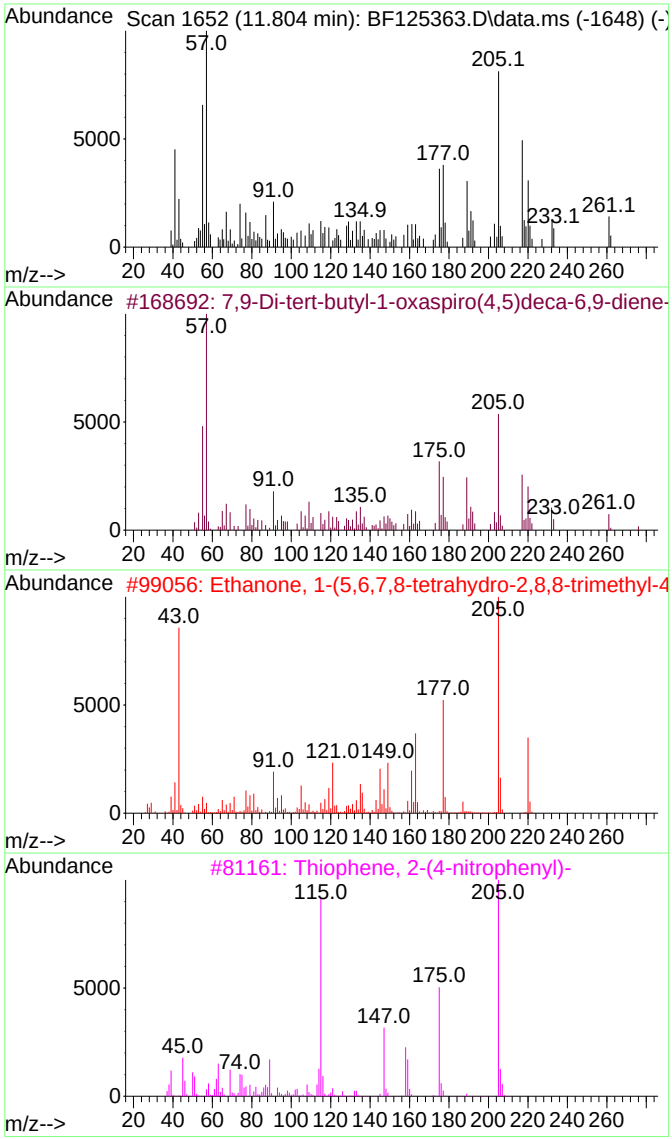
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

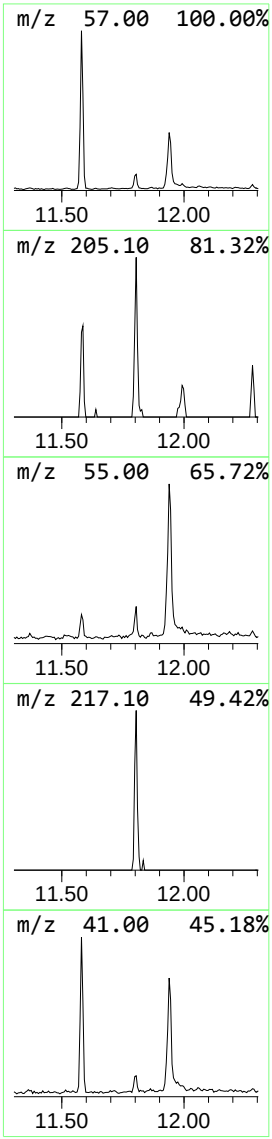
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.28 ng	112065	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	49
3	Thiophene, 2-(4-nitrophenyl)-	205	C10H7NO2S	059156-21-7	46
4	2,6-Bis(1,1-dimethylethyl)-4-met...	262	C18H30O	004278-82-4	46
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

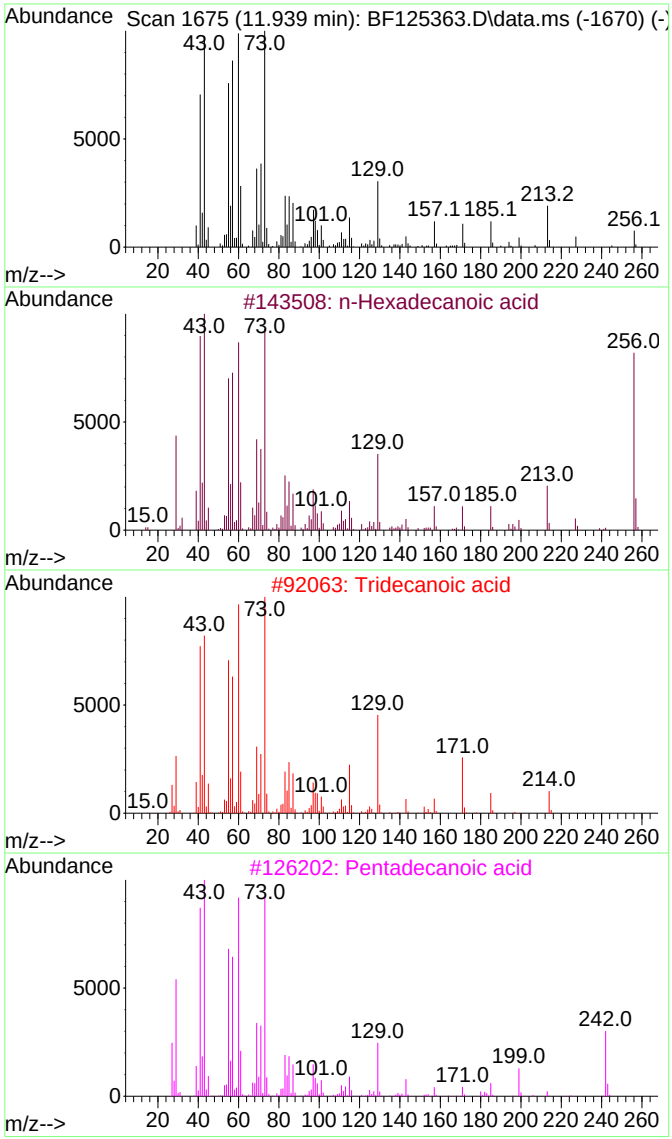
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

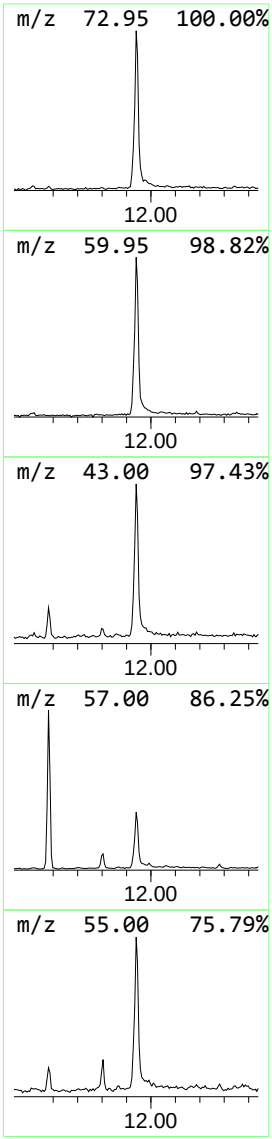
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	13.01 ng	638156	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

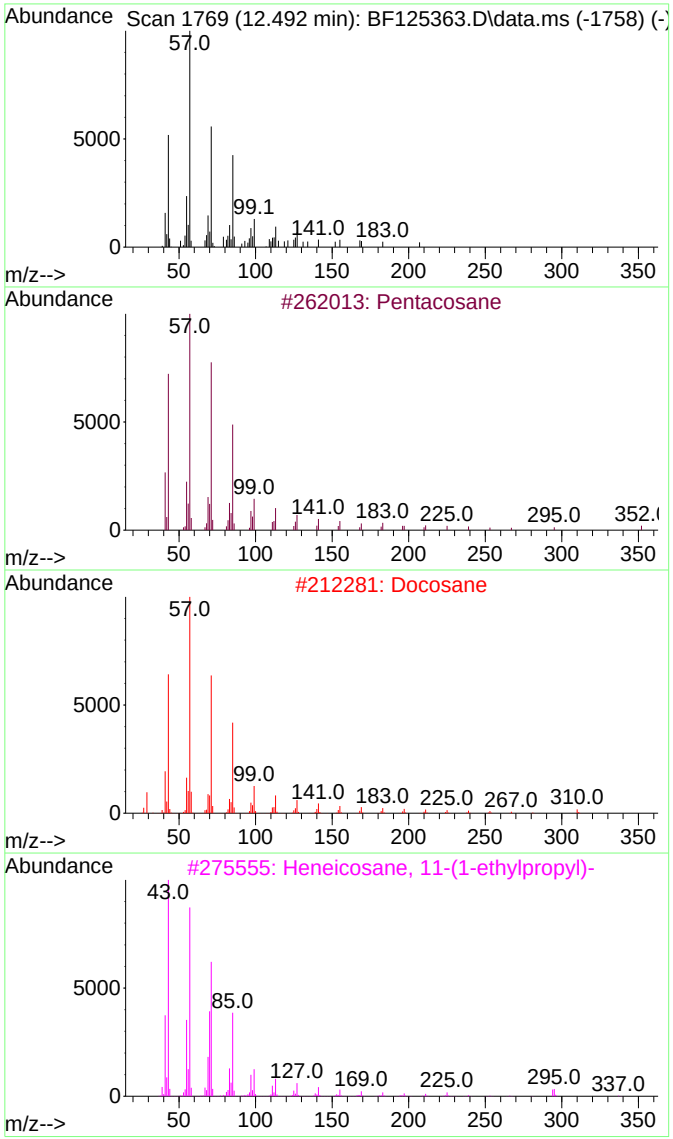
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

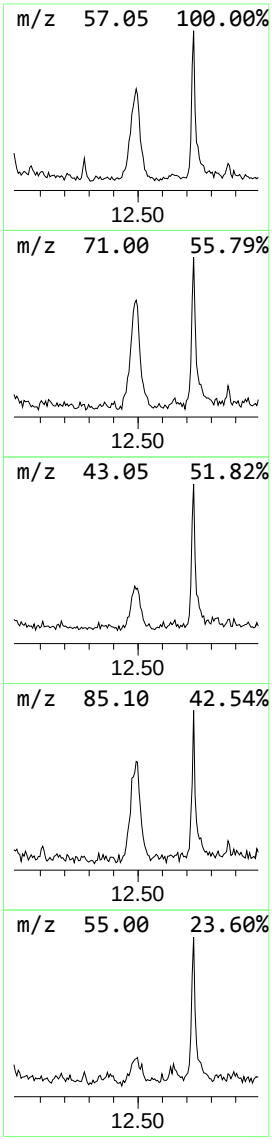
****

Peak Number 5 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	3.66 ng	179767	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Docosane	310	C22H46	000629-97-0	86
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5	Octadecane	254	C18H38	000593-45-3	86





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Sample : M3648-10
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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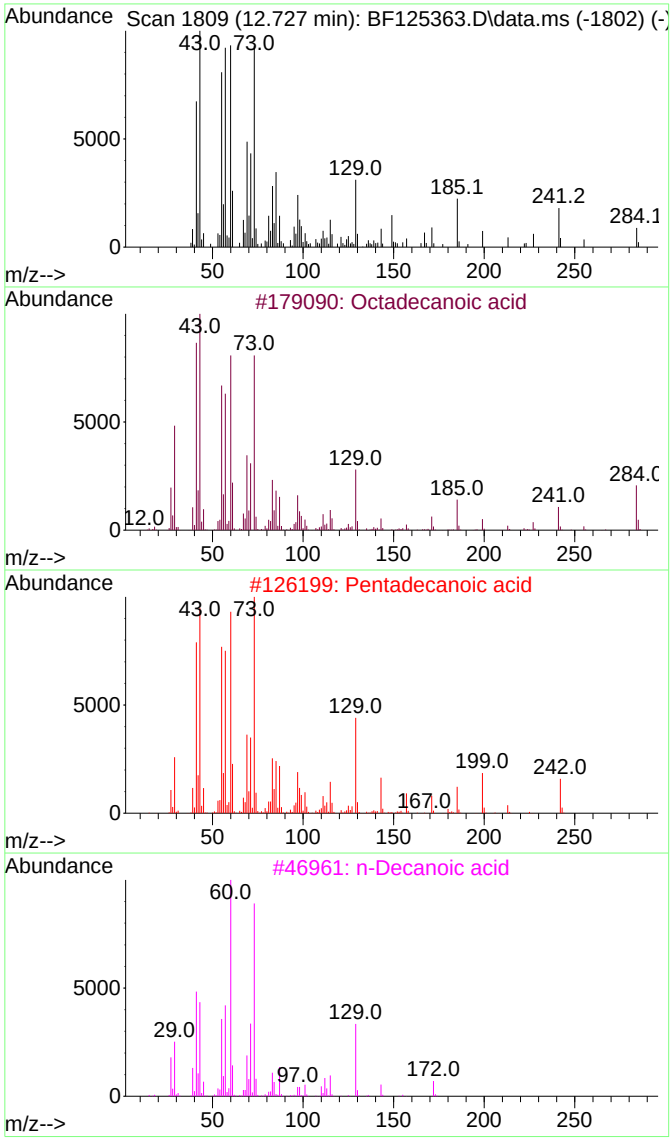
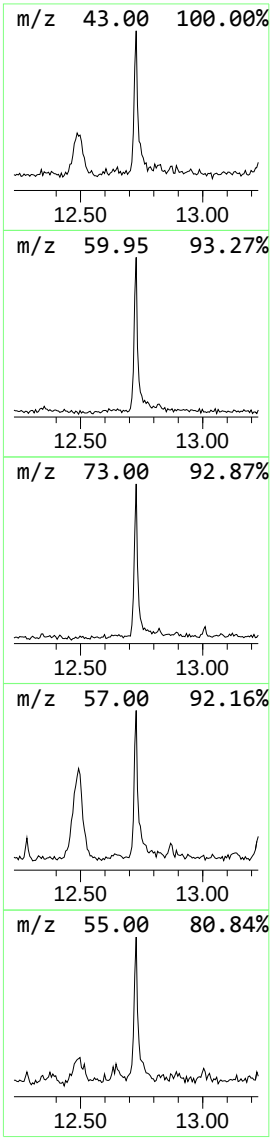
Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	7.32 ng	359169	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46





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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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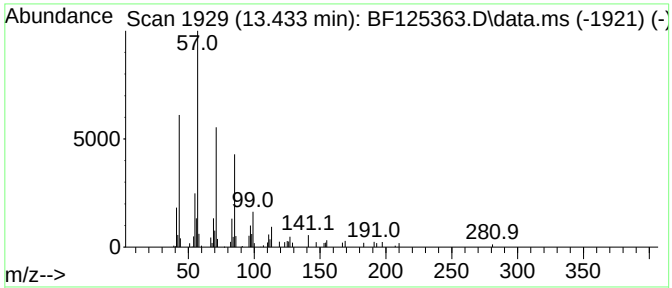
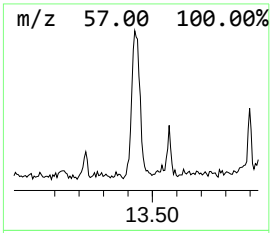
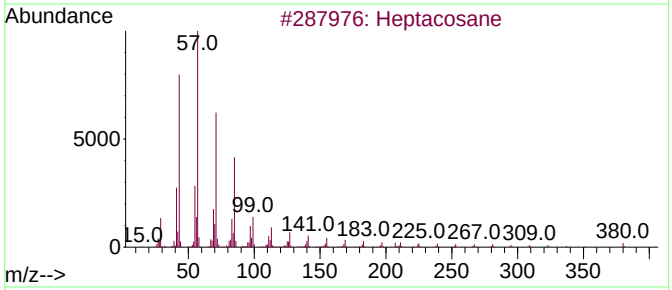
Peak Number 7 Heptacosane Concentration Rank 5

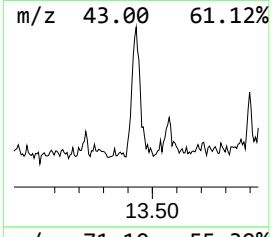
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	6.58 ng	237506	Chrysene-d12	14.063

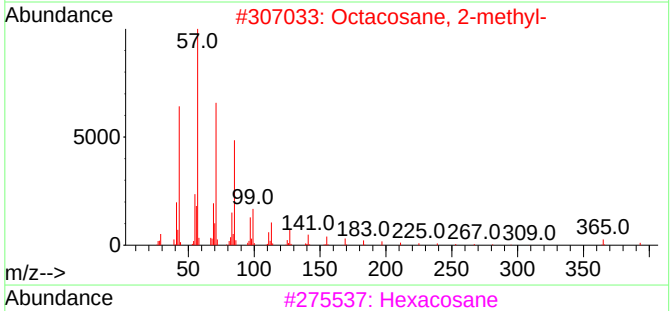
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Octacosane	394	C28H58	000630-02-4	91

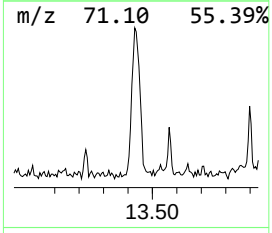


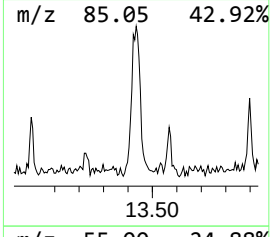


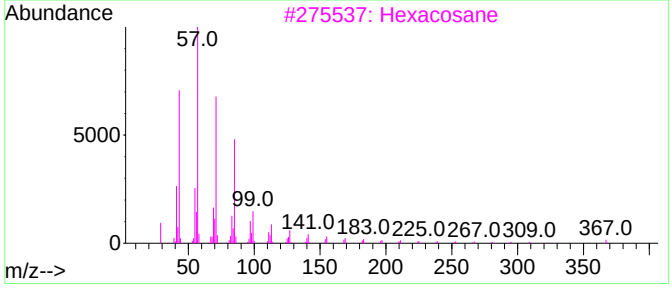


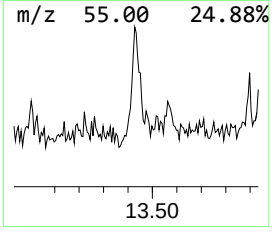












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Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

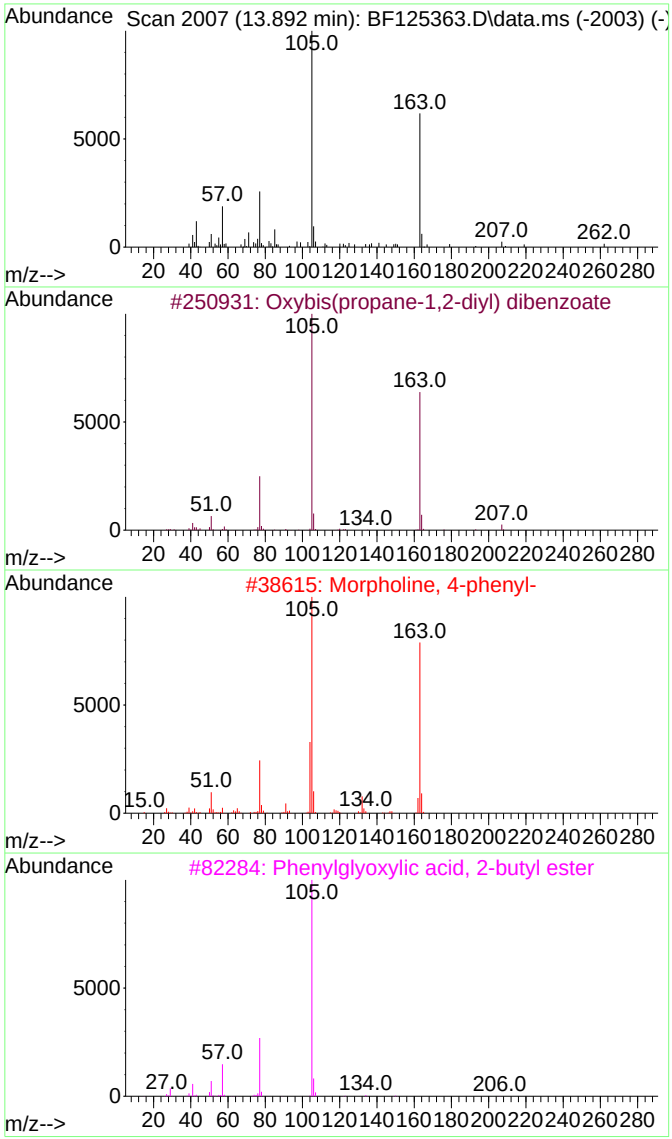
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

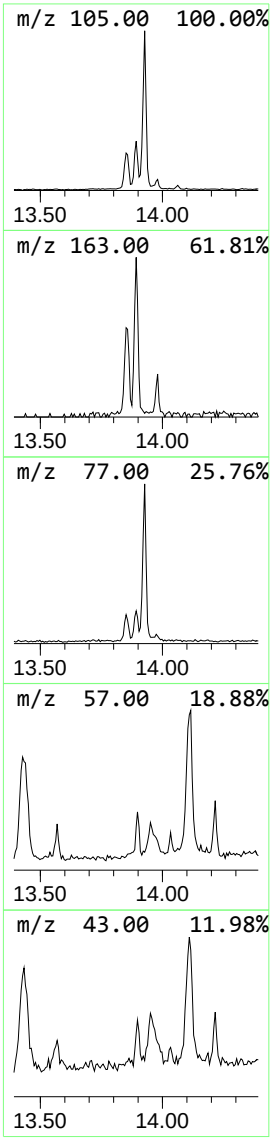
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Oxybis(propane-1,2-diyl) di... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.68 ng	96872	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	Phenylglyoxylic acid, 2-butyl ester	206	C12H14O3	1000453-46-5	38
4	3-Benzoyl-2-t-butyl-4-vinyl-oxaz...	273	C16H19NO3	109918-60-7	35
5	3-Benzoyl-2-t-butyl-4-isopropyl-...	303	C18H25NO3	104057-75-2	35





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Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

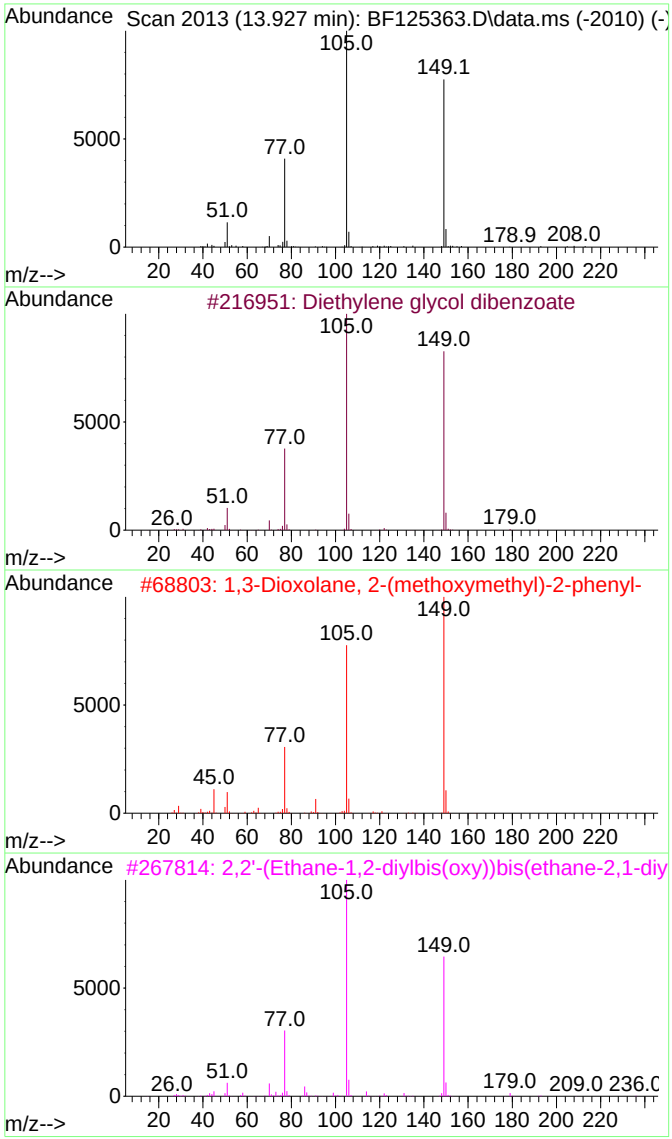
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

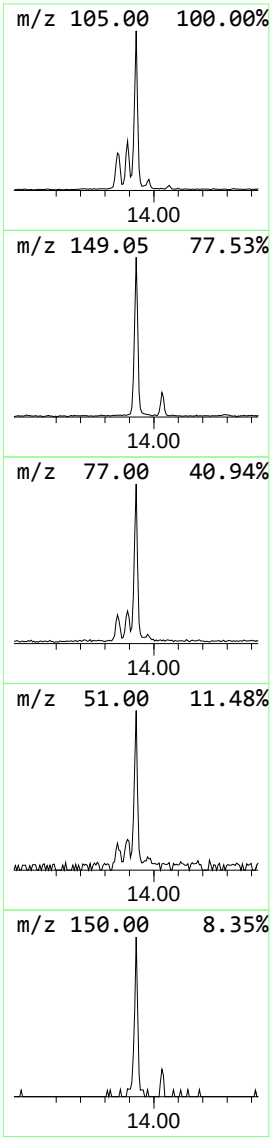
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	5.77 ng	208383	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	47
4	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	43
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43





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Sample : M3648-10
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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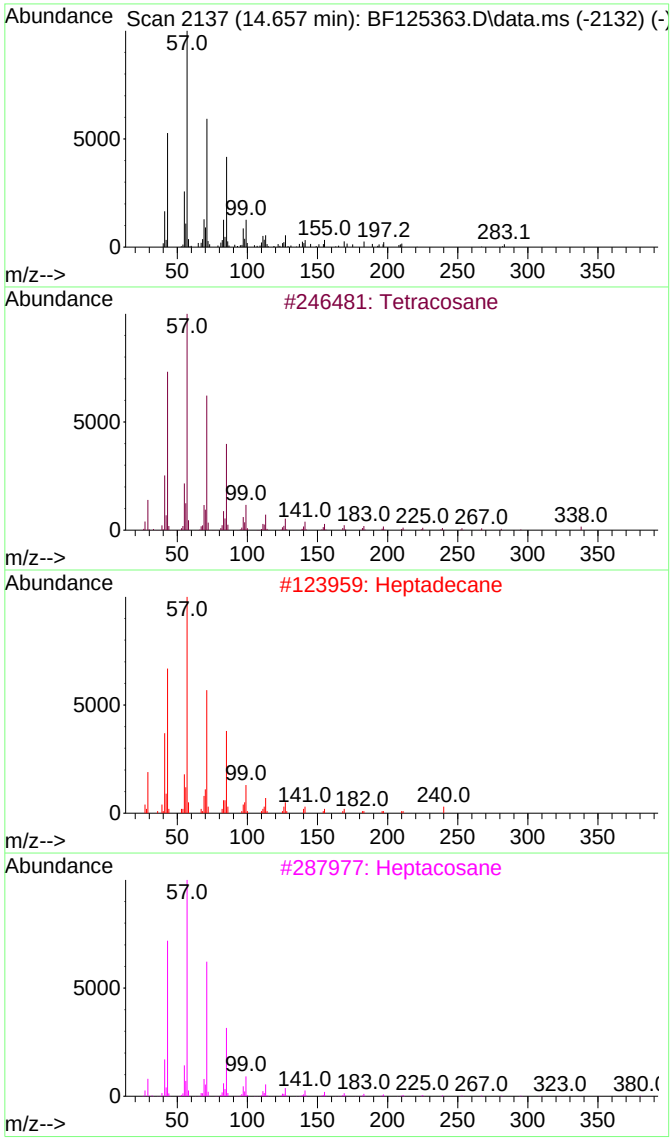
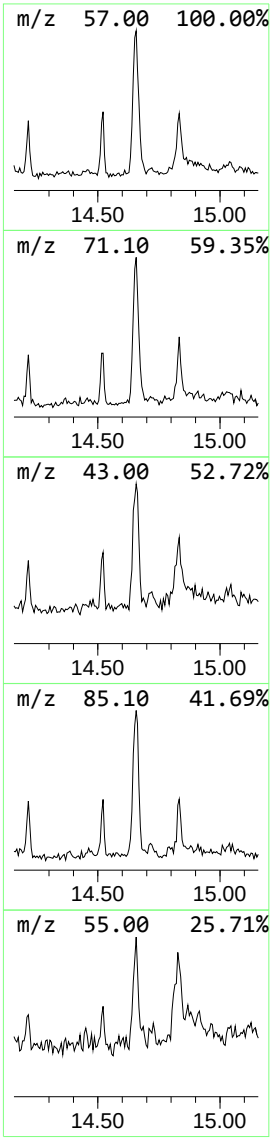
Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	5.48 ng	197896	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Heptadecane	240	C17H36	000629-78-7	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Hexadecane	226	C16H34	000544-76-3	86





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Sample : M3648-10
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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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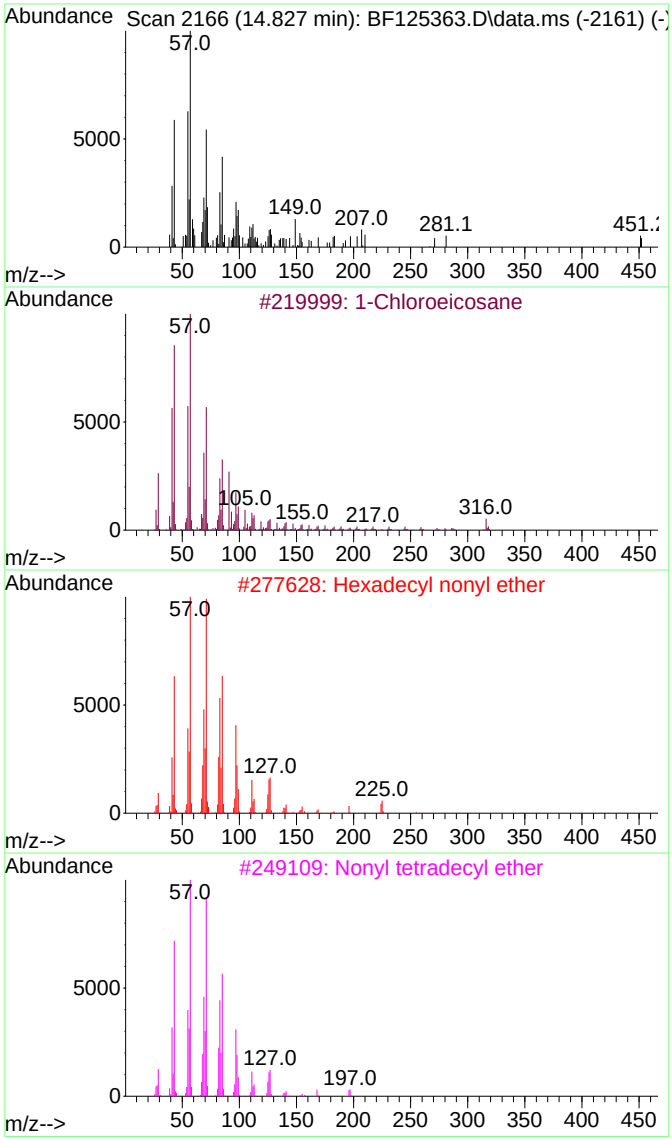
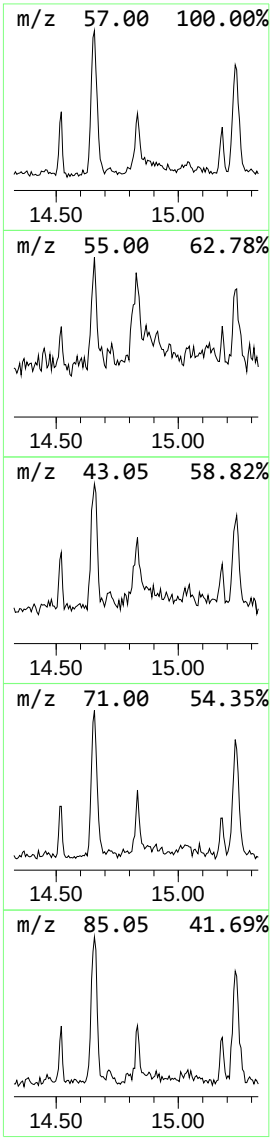
Peak Number 11 1-Chloroeicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	2.81 ng	117411	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	64
2	Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	62
3	Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	62
4	Dodecyl nonyl ether	312	C21H44O	1000406-37-5	58
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	58





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Operator : JU/CG
Sample : M3648-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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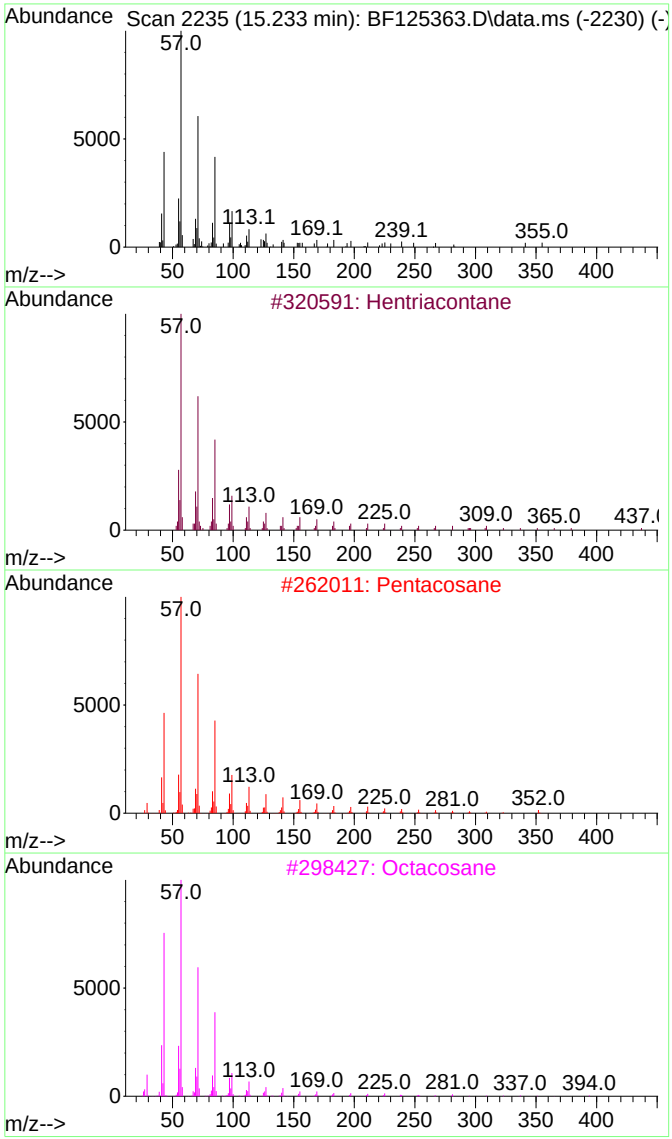
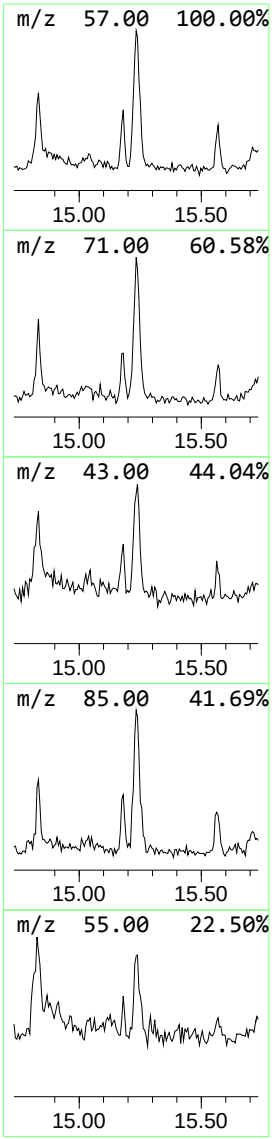
Peak Number 12 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	3.69 ng	154030	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Pentacosane	352	C25H52	000629-99-2	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	86





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Operator : JU/CG
Sample : M3648-10
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Instrument :
BNA_F
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TIC Integration Parameters: LSCINT.P

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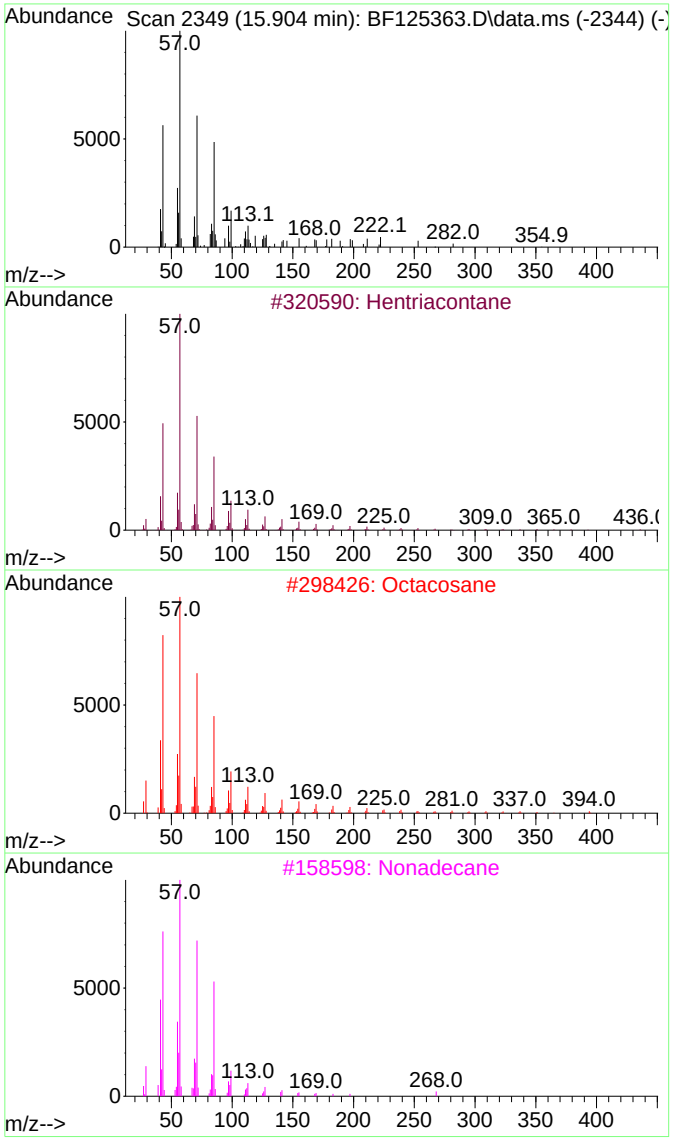
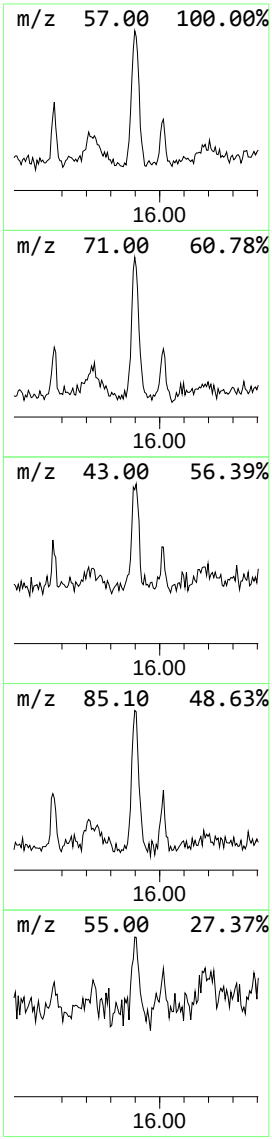
Peak Number 13 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.904	3.00 ng	125595	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	86
2	Octacosane	394	C28H58	000630-02-4	80
3	Nonadecane	268	C19H40	000629-92-5	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72





Tentatively Identified Compound (LSC) summary

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Data File : BF125363.D
Acq On : 4 Sep 2021 11:51
Operator : JU/CG
Sample : M3648-10
Misc :
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Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.187	85.7	ng	3418290	1	6.898	797412	20.0
1,2-Benzenedica...	11.580	14.4	ng	706153	4	11.422	981174	20.0
7,9-Di-tert-but...	11.804	2.3	ng	112065	4	11.422	981174	20.0
n-Hexadecanoic ...	11.939	13.0	ng	638156	4	11.422	981174	20.0
Pentacosane	12.492	3.7	ng	179767	4	11.422	981174	20.0
Octadecanoic acid	12.727	7.3	ng	359169	4	11.422	981174	20.0
Heptacosane	13.433	6.6	ng	237506	5	14.063	722050	20.0
Oxybis(propane-...	13.892	2.7	ng	96872	5	14.063	722050	20.0
Diethylene glyc...	13.927	5.8	ng	208383	5	14.063	722050	20.0
Tetracosane	14.657	5.5	ng	197896	5	14.063	722050	20.0
1-Chloroeicosane	14.827	2.8	ng	117411	6	15.557	835937	20.0
Hentriacontane	15.233	3.7	ng	154030	6	15.557	835937	20.0
Octacosane	15.904	3.0	ng	125595	6	15.557	835937	20.0