LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134368.D
Acq On : 19 Jul 2023 20:18
Operator : CG\JU
Sample : 03641-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP13

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB	316732	365747	24.77%	3.215%
2	5.475	572	576	592	rBV	1351890	1216821	82.40%	10.695%
3	6.481	742	747	762	rBV	1260320	1235490	83.66%	10.859%
4	6.834	804	807	817	rBV	440332	405425	27.45%	3.563%
5	7.398	899	903	906	rBV	887209	763746	51.72%	6.713%
6	8.116	1021	1025	1028	rBV	658890	505642	34.24%	4.444%
7	9.192	1204	1208	1211	rBV	1964295	1476789	100.00%	12.980%
8	9.875	1320	1324	1327	rBV	610486	524053	35.49%	4.606%
9	10.669	1455	1459	1475	rBV	939627	867227	58.72%	7.622%
10	11.369	1574	1578	1580	rBV	563495	470810	31.88%	4.138%
11	11.392	1580	1582	1586	rVB	61189	49562	3.36%	0.436%
12	11.863	1659	1662	1665	rBV3	22642	30622	2.07%	0.269%
13	11.898	1665	1668	1675	rVV3	265481	242770	16.44%	2.134%
14	12.586	1782	1785	1788	rBV	159431	149556	10.13%	1.315%
15	12.686	1800	1802	1808	rBV2	45983	50659	3.43%	0.445%
16	12.822	1819	1825	1829	rBV	145645	144436	9.78%	1.270%
17	12.963	1845	1849	1853	rBV	1434041	1185017	80.24%	10.416%
18	13.151	1878	1881	1885	rVB	19741	20303	1.37%	0.178%
19	13.533	1942	1946	1949	rBV2	20609	22367	1.51%	0.197%
20	13.669	1961	1969	1972	rBV4	14515	25077	1.70%	0.220%
21	13.892	2000	2007	2015	rBV6	51763	136457	9.24%	1.199%
22	14.027	2022	2030	2033	rBV2	462684	502251	34.01%	4.415%
23	14.057	2033	2035	2042	rVB	76898	71076	4.81%	0.625%
24	14.121	2043	2046	2051	rVB2	25876	32590	2.21%	0.286%
25	14.186	2054	2057	2061	rBV2	29898	28307	1.92%	0.249%
26	14.492	2106	2109	2112	rBV2	29738	28652	1.94%	0.252%
27	14.963	2185	2189	2195	rVB2	42275	49749	3.37%	0.437%
28	15.092	2207	2211	2219	rBV	64093	124980	8.46%	1.099%
29	15.157	2219	2222	2227	rVB3	34608	42602	2.88%	0.374%
30	15.239	2232	2236	2242	rVB7	15597	31358	2.12%	0.276%
31	15.404	2261	2264	2269	rVB	32478	42990	2.91%	0.378%
32	15.468	2272	2275	2281	rVB	44422	56919	3.85%	0.500%
33	15.533	2281	2286	2299	rBV	228654	352384	23.86%	3.097%
34	15.763	2323	2325	2330	rVB6	15827	19383	1.31%	0.170%
35	16.010	2363	2367	2373	rVB	35039	50862	3.44%	0.447%
36	17.039	2537	2542	2544	rBV6	9178	19301	1.31%	0.170%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134368.D
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP13

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.086	2546	2550	2557	rVB3	16721	35275	2.39%	0.310%

Sum of corrected areas: 11377255

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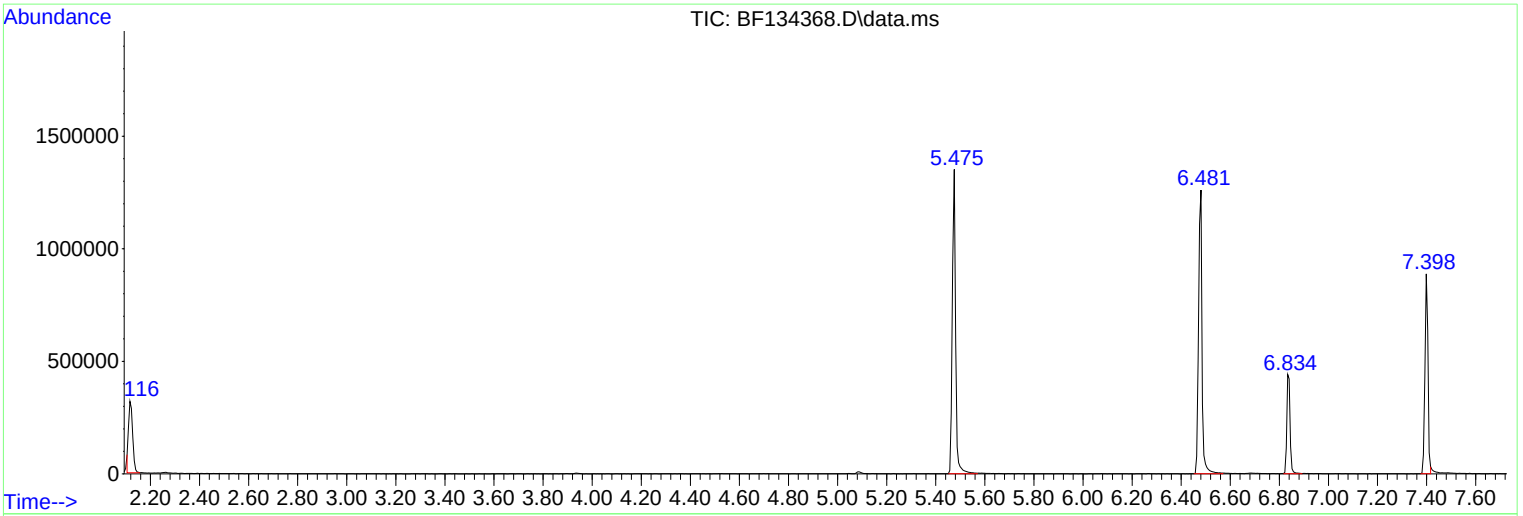
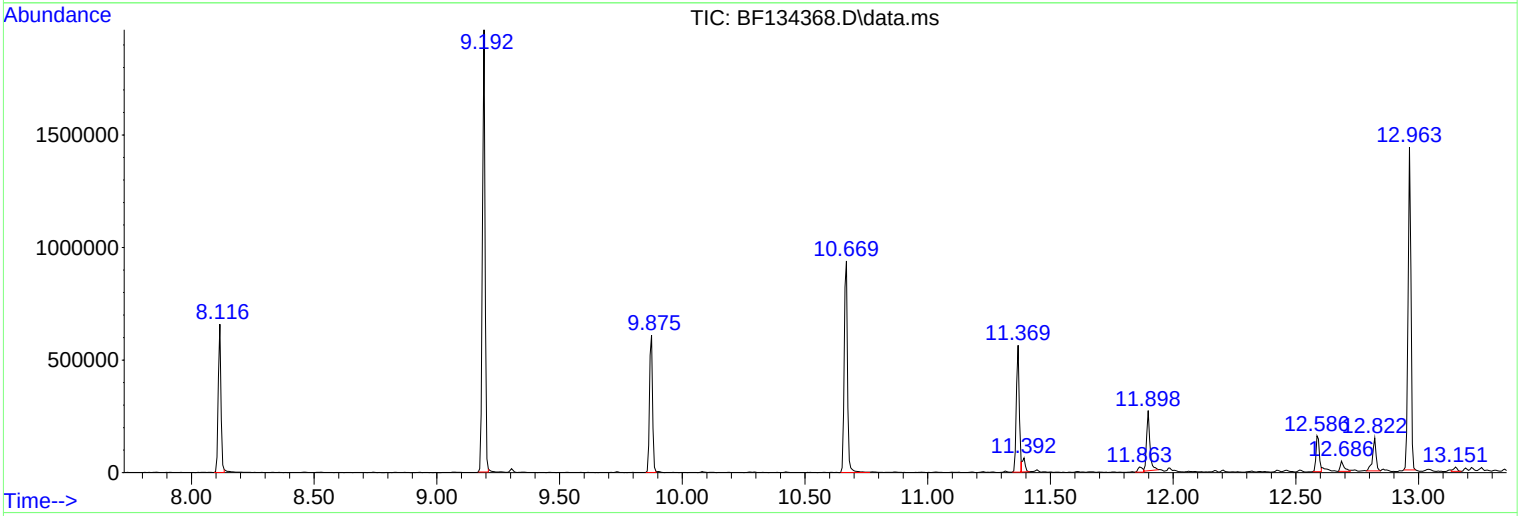
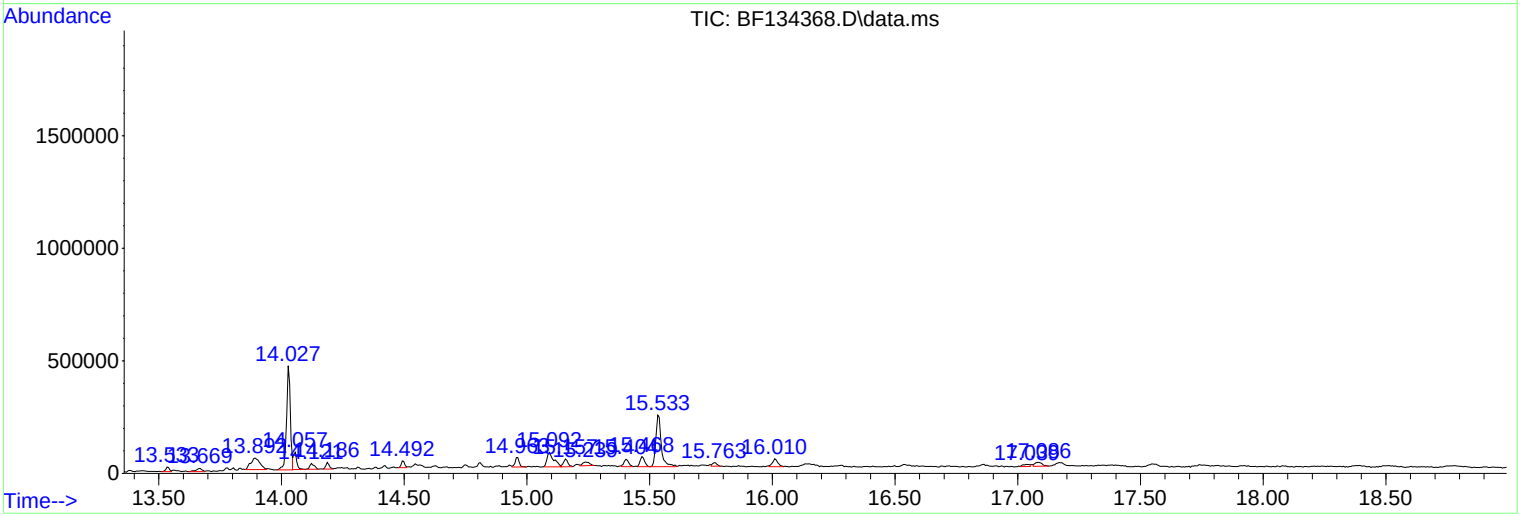
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

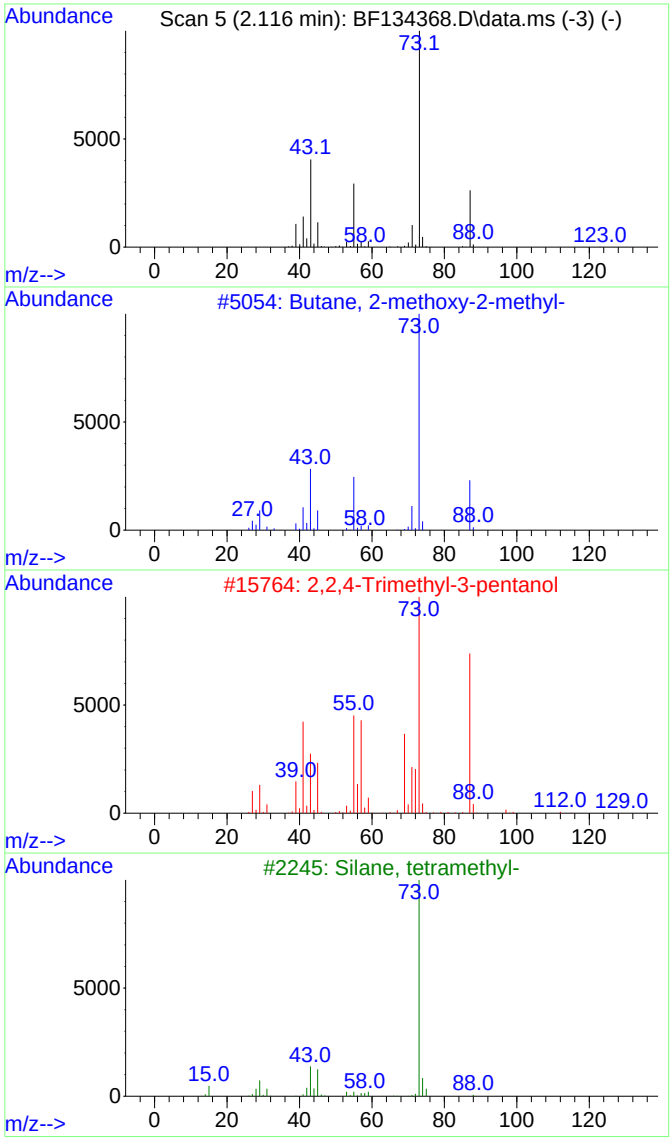
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

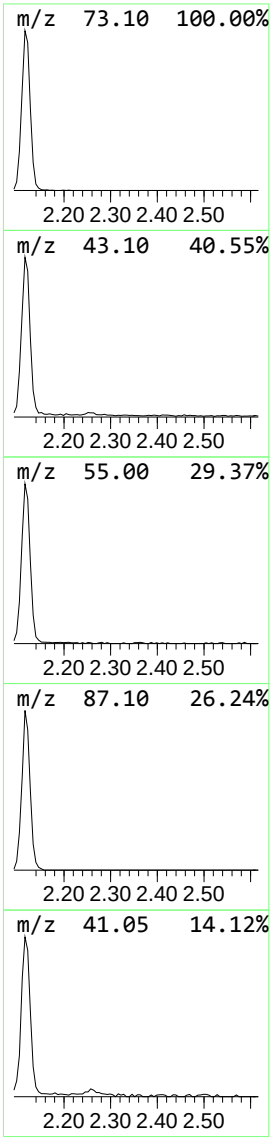
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	18.04 ng	365747	1,4-Dichlorobenzene-d4	6.840

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	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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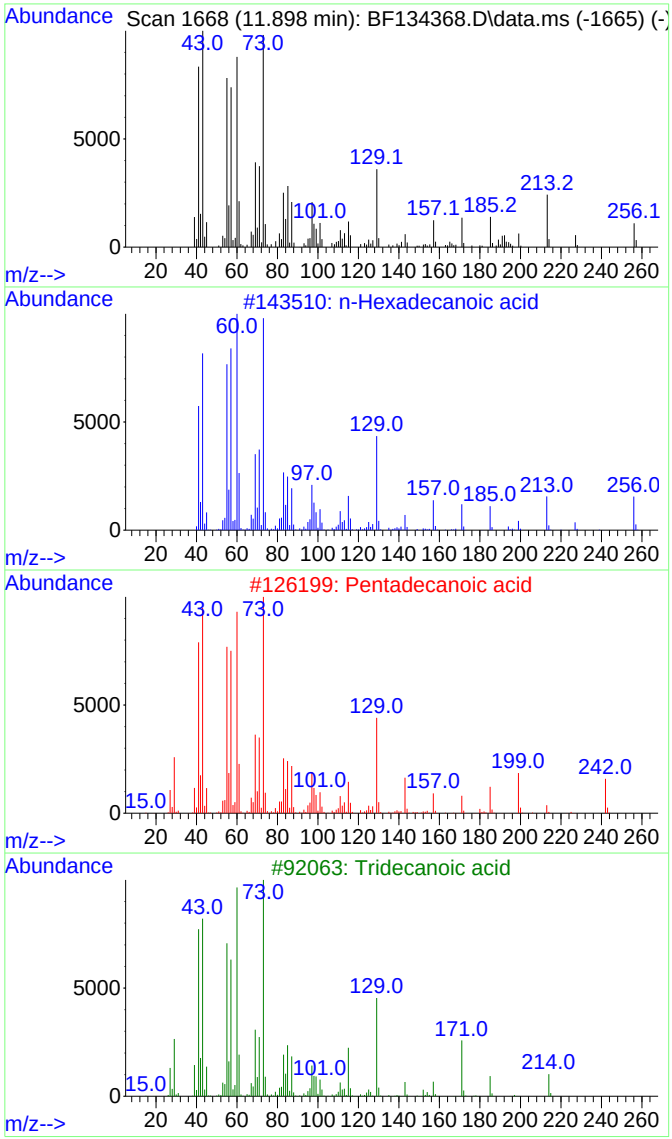
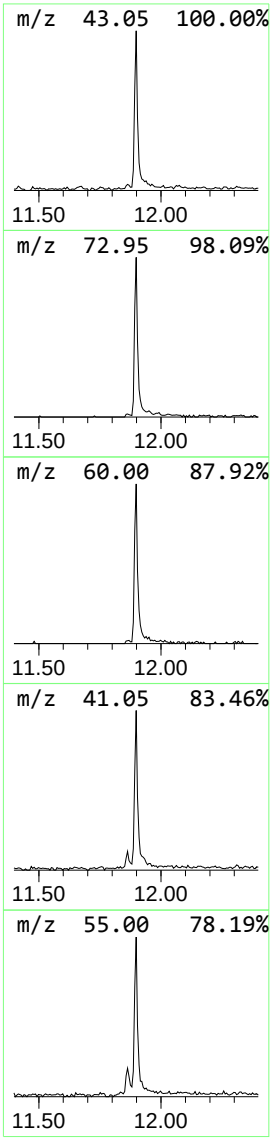
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	10.31 ng	242770	Phenanthrene-d10	11.369

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	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Data File : BF134368.D
Acq On : 19 Jul 2023 20:18
Operator : CG\JU
Sample : 03641-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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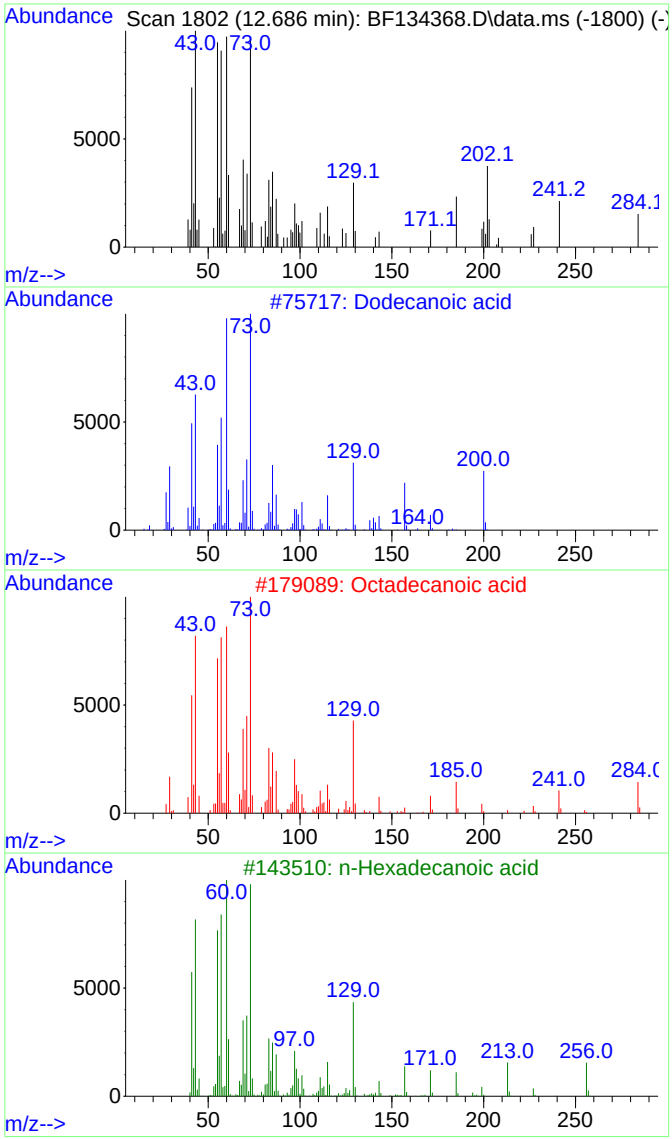
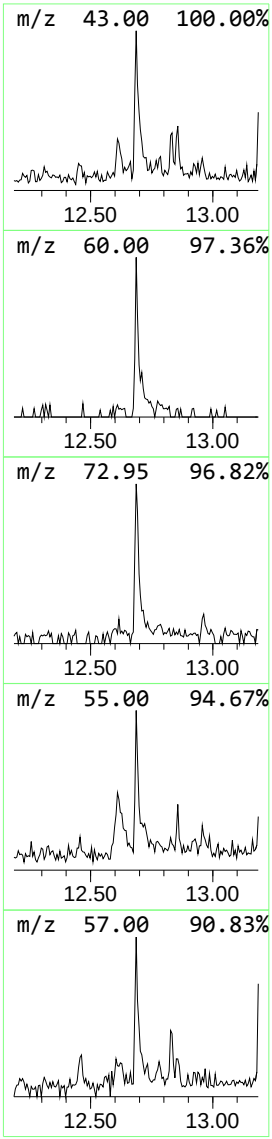
Peak Number 3 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	2.15 ng	50659	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	92
2	Octadecanoic acid	284	C18H36O2	000057-11-4	70
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





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Acq On : 19 Jul 2023 20:18
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Sample : 03641-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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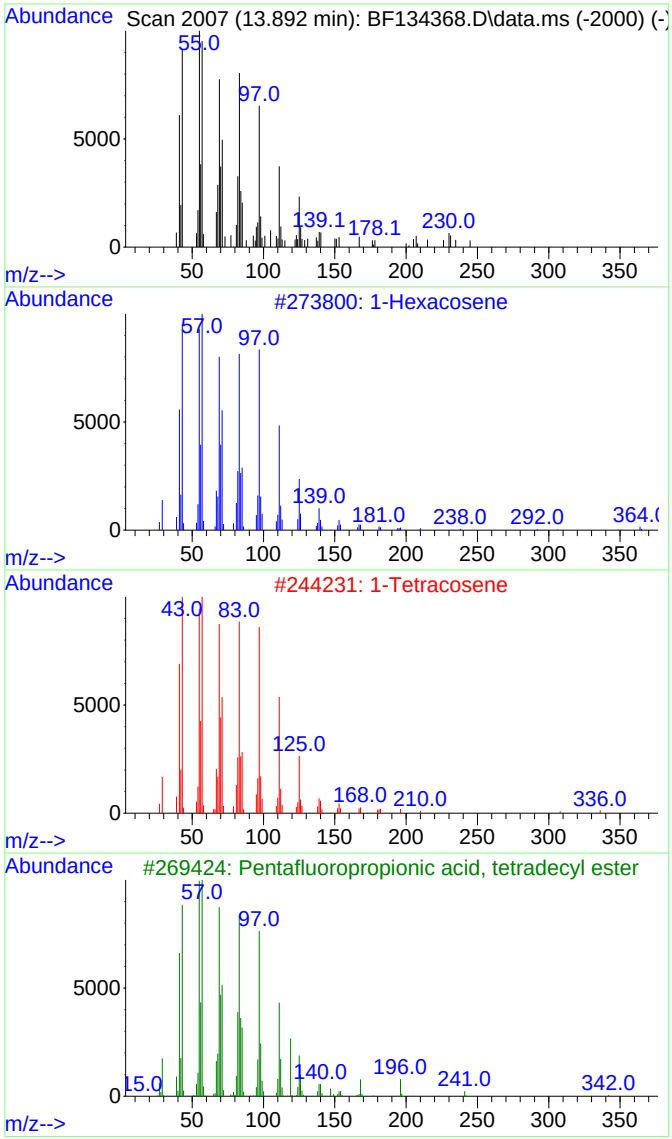
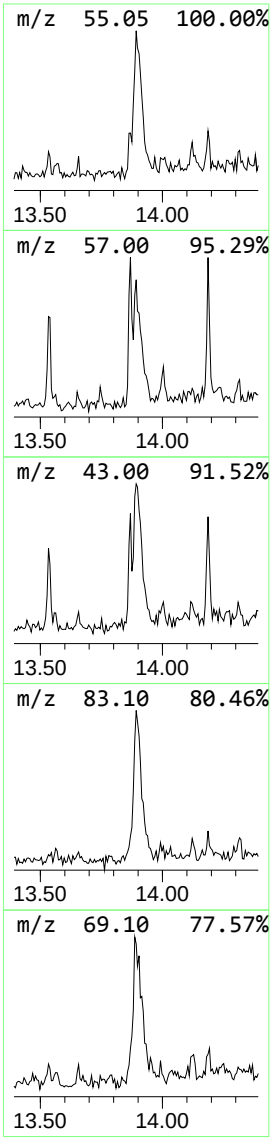
Peak Number 4 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.43 ng	136457	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	1-Tetracosene	336	C24H48	010192-32-2	94
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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Sample : 03641-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

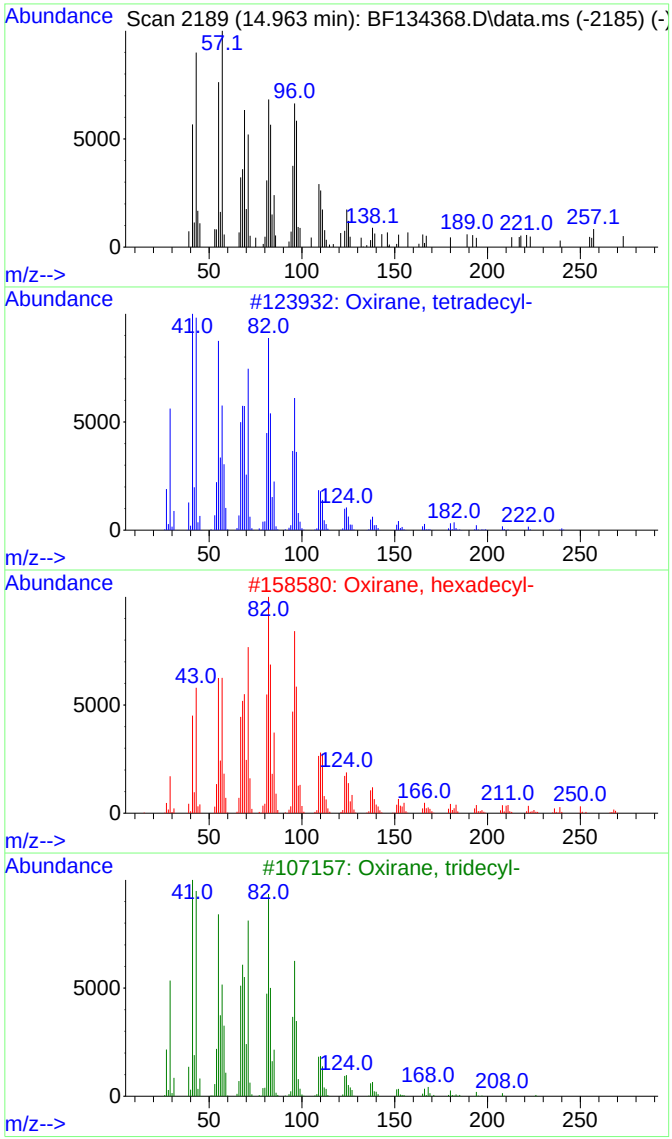
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

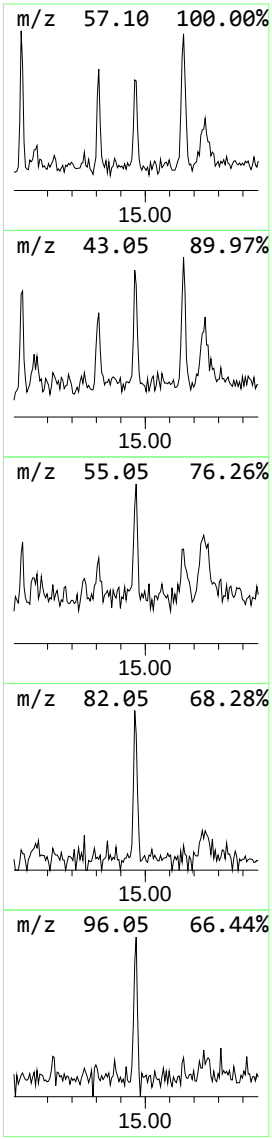
****

Peak Number 5 Oxirane, tetradecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	2.82 ng	49749	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	87
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3	Oxirane, tridecyl-	226	C15H30O	018633-25-5	83
4	1,19-Eicosadiene	278	C20H38	014811-95-1	68
5	Octadecanal	268	C18H36O	000638-66-4	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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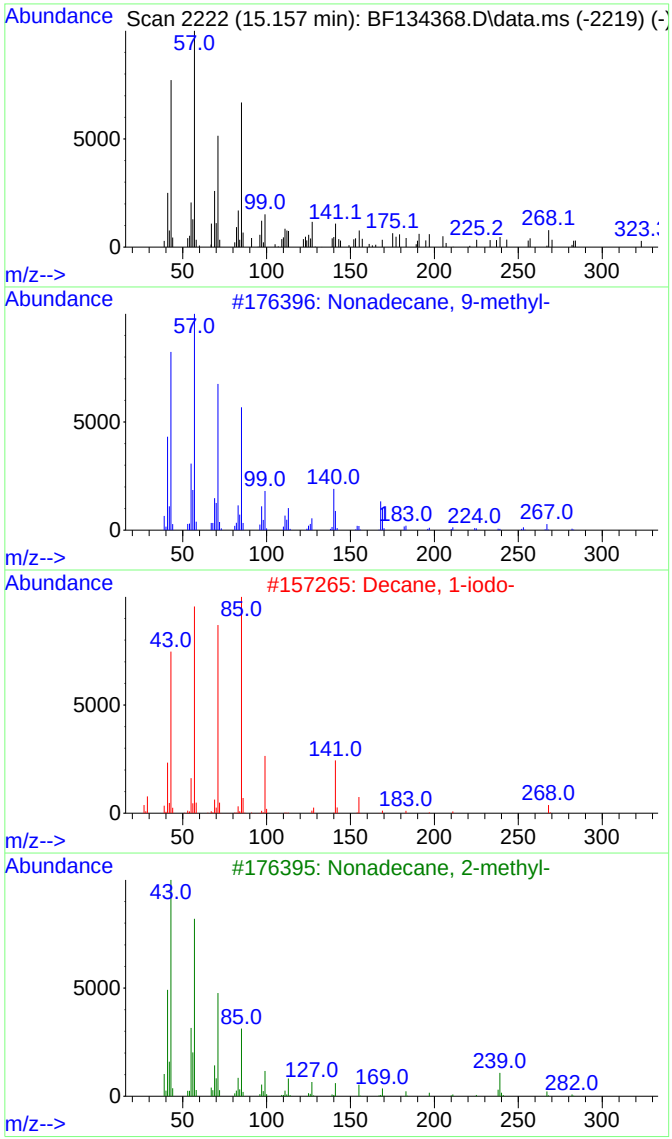
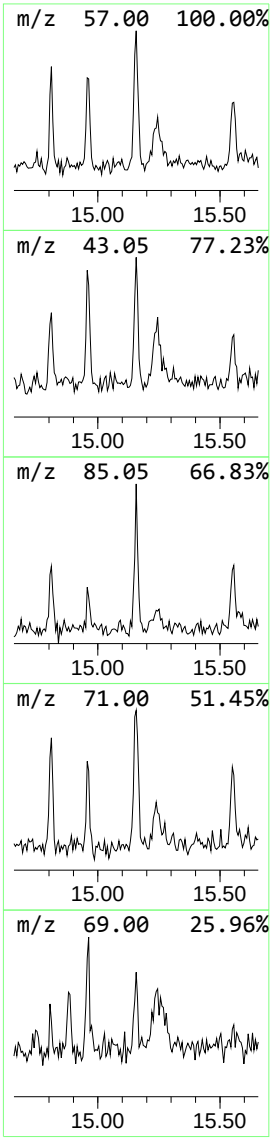
Peak Number 6 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	2.42 ng	42602	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
2	Decane, 1-iodo-	268	C10H21I	002050-77-3	81
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	64
4	1-Trifluorosilyltridecane	268	C13H27F3Si	1010217-08-2	62
5	Nonadecane	268	C19H40	000629-92-5	62





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ALS Vial : 15 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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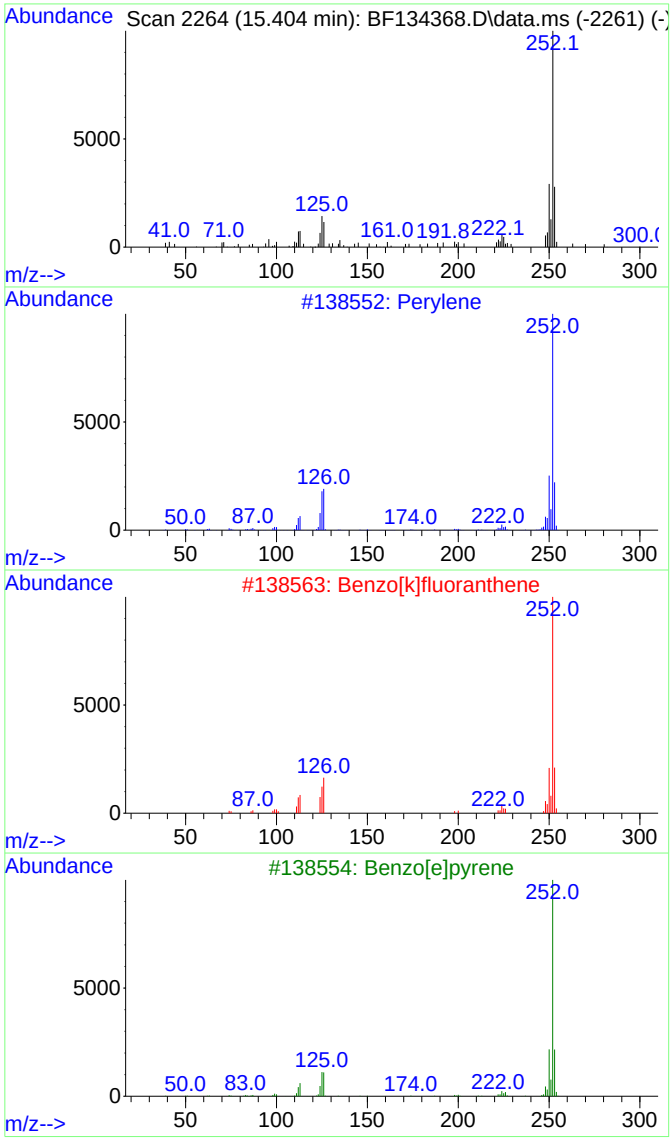
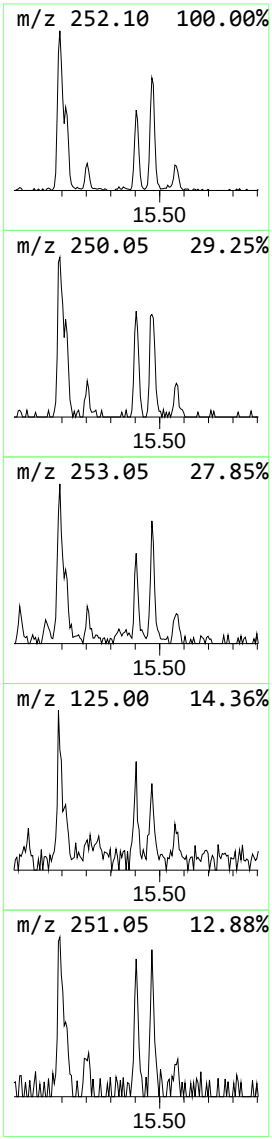
Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.44 ng	42990	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
3	Benzo[e]pyrene	252	C20H12	000192-97-2	81
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	76





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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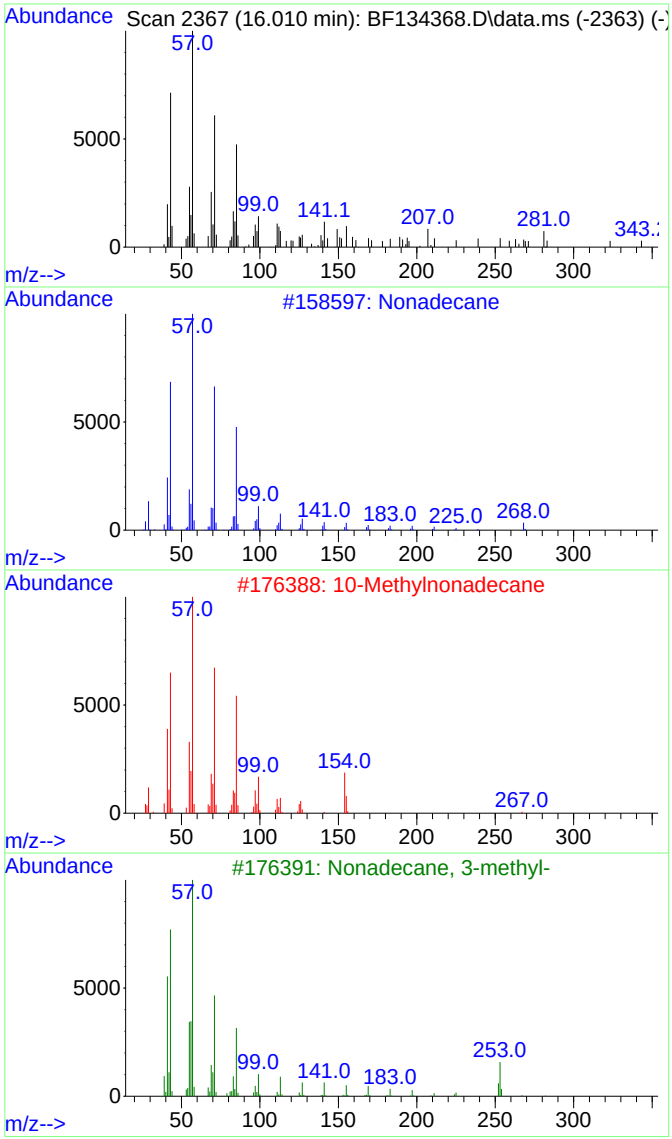
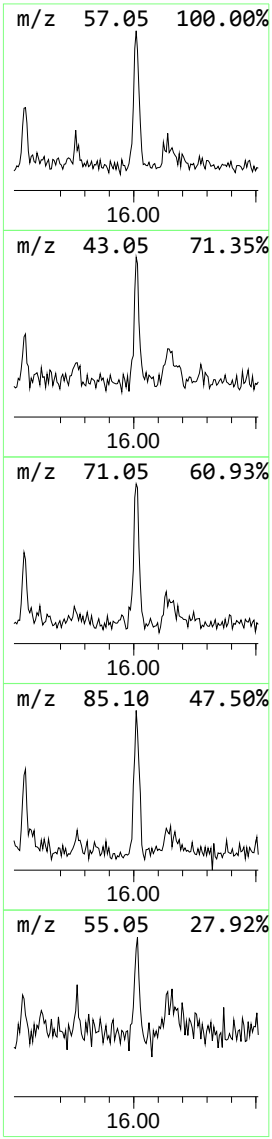
Peak Number 8 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.89 ng	50862	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	92
2	10-Methylnonadecane	282	C20H42	056862-62-5	70
3	Nonadecane, 3-methyl-	282	C20H42	006418-45-7	70
4	Heptacosane	380	C27H56	000593-49-7	58
5	Tetracosane	338	C24H50	000646-31-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134368.D
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Instrument :
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ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.116	18.0	ng	365747	1	6.840	405425	20.0
n-Hexadecanoic ...	11.898	10.3	ng	242770	4	11.369	470810	20.0
Dodecanoic acid	12.686	2.1	ng	50659	4	11.369	470810	20.0
1-Hexacosene	13.892	5.4	ng	136457	5	14.027	502251	20.0
Oxirane, tetrad...	14.963	2.8	ng	49749	6	15.533	352384	20.0
Nonadecane, 9-m...	15.157	2.4	ng	42602	6	15.533	352384	20.0
Perylene	15.404	2.4	ng	42990	6	15.533	352384	20.0
Nonadecane	16.010	2.9	ng	50862	6	15.533	352384	20.0