LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140276.D
Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-110424

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	21	rVB	1291049	2017832	67.80%	7.316%
2	2.246	21	26	39	rVB	38683	70233	2.36%	0.255%
3	5.087	500	509	519	rBV	317398	482780	16.22%	1.750%
4	5.492	571	578	583	rBV	1761681	2357912	79.23%	8.549%
5	5.892	640	646	652	rVB	27955	37910	1.27%	0.137%
6	6.498	742	749	754	rBV	1784431	2416108	81.18%	8.760%
7	6.875	808	813	818	rBV	660703	798586	26.83%	2.895%
8	7.433	902	908	913	rBV	1279044	1608506	54.05%	5.832%
9	8.157	1025	1031	1040	rBV	811148	1027218	34.52%	3.724%
10	9.233	1208	1214	1219	rBV	2355234	2976111	100.00%	10.790%
11	9.774	1301	1306	1311	rBV	30890	43451	1.46%	0.158%
12	9.916	1324	1330	1334	rBV	860260	1118300	37.58%	4.054%
13	10.463	1419	1423	1428	rVB	23488	33016	1.11%	0.120%
14	10.627	1446	1451	1458	rVB	113546	146747	4.93%	0.532%
15	10.704	1458	1464	1476	rVV	1182438	1581555	53.14%	5.734%
16	10.827	1480	1485	1491	rVB4	26295	47013	1.58%	0.170%
17	11.404	1577	1583	1591	rBV2	736094	1179707	39.64%	4.277%
18	11.474	1591	1595	1599	rVB	47556	63067	2.12%	0.229%
19	11.633	1618	1622	1629	rBV2	17152	34349	1.15%	0.125%
20	11.933	1663	1673	1679	rBV	309515	545515	18.33%	1.978%
21	12.016	1683	1687	1695	rVB	76652	145441	4.89%	0.527%
22	12.457	1758	1762	1765	rBV	32578	48337	1.62%	0.175%
23	12.492	1765	1768	1773	rVV2	28610	43953	1.48%	0.159%
24	12.615	1784	1789	1794	rBV	425281	553795	18.61%	2.008%
25	12.715	1802	1806	1813	rBV2	43912	71682	2.41%	0.260%
26	12.845	1821	1828	1834	rBV	386796	585900	19.69%	2.124%
27	12.992	1846	1853	1860	rVB	1687533	2212371	74.34%	8.021%
28	13.063	1861	1865	1873	rBV4	36195	72300	2.43%	0.262%
29	13.174	1877	1884	1888	rBV2	73060	125995	4.23%	0.457%
30	13.239	1892	1895	1898	rVV	55270	74558	2.51%	0.270%
31	13.280	1898	1902	1910	rVB	45036	71044	2.39%	0.258%
32	13.798	1986	1990	1992	rBV3	49037	75235	2.53%	0.273%
33	13.898	2003	2007	2016	rVB5	164063	335720	11.28%	1.217%
34	14.045	2026	2032	2036	rBV2	761247	1279688	43.00%	4.640%
35	14.521	2110	2113	2115	rBV2	54764	76629	2.57%	0.278%
36	14.980	2188	2191	2199	rVB	124765	182051	6.12%	0.660%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140276.D
Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.104	2207	2212	2220	rBV	246124	526106	17.68%	1.907%
38	15.180	2221	2225	2227	rBV	107700	156510	5.26%	0.567%
39	15.221	2228	2232	2243	rVV3	98360	323904	10.88%	1.174%
40	15.409	2260	2264	2270	rVB	134180	214493	7.21%	0.778%
41	15.474	2270	2275	2280	rBV	208594	390164	13.11%	1.415%
42	15.539	2281	2286	2297	rVB2	421566	813581	27.34%	2.950%
43	15.774	2323	2326	2332	rVB3	88424	139988	4.70%	0.508%
44	16.015	2363	2367	2374	rVB	116882	218033	7.33%	0.790%
45	16.845	2503	2508	2520	rVB4	98909	258430	8.68%	0.937%

Sum of corrected areas: 27581824

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
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Instrument :
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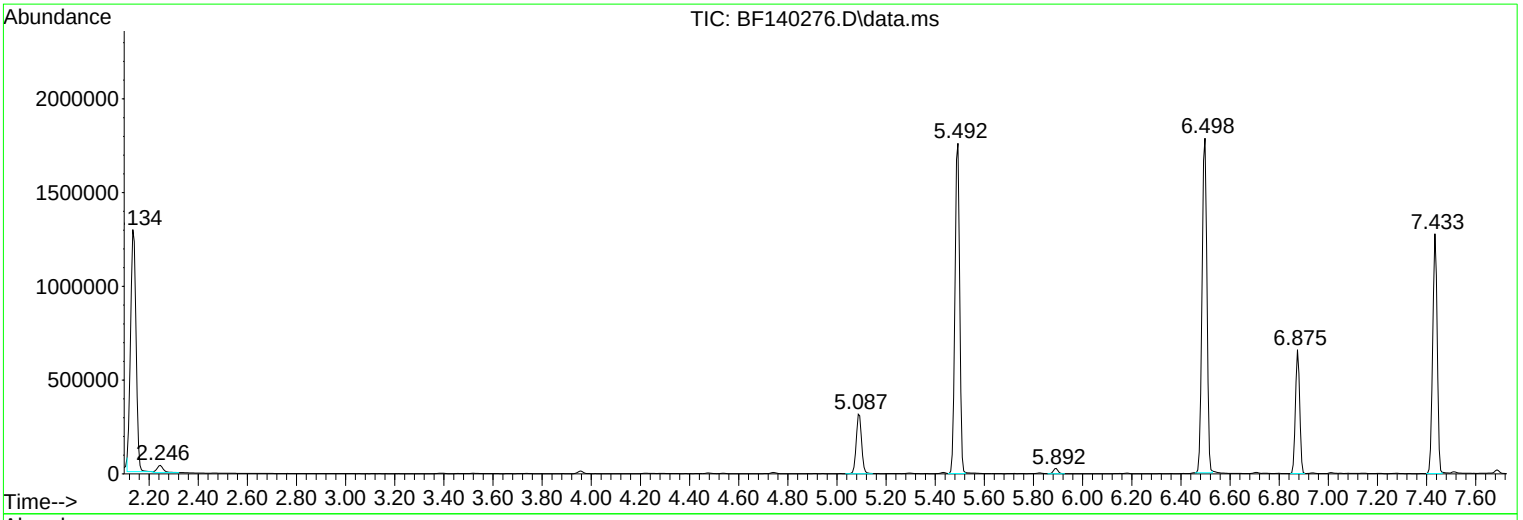
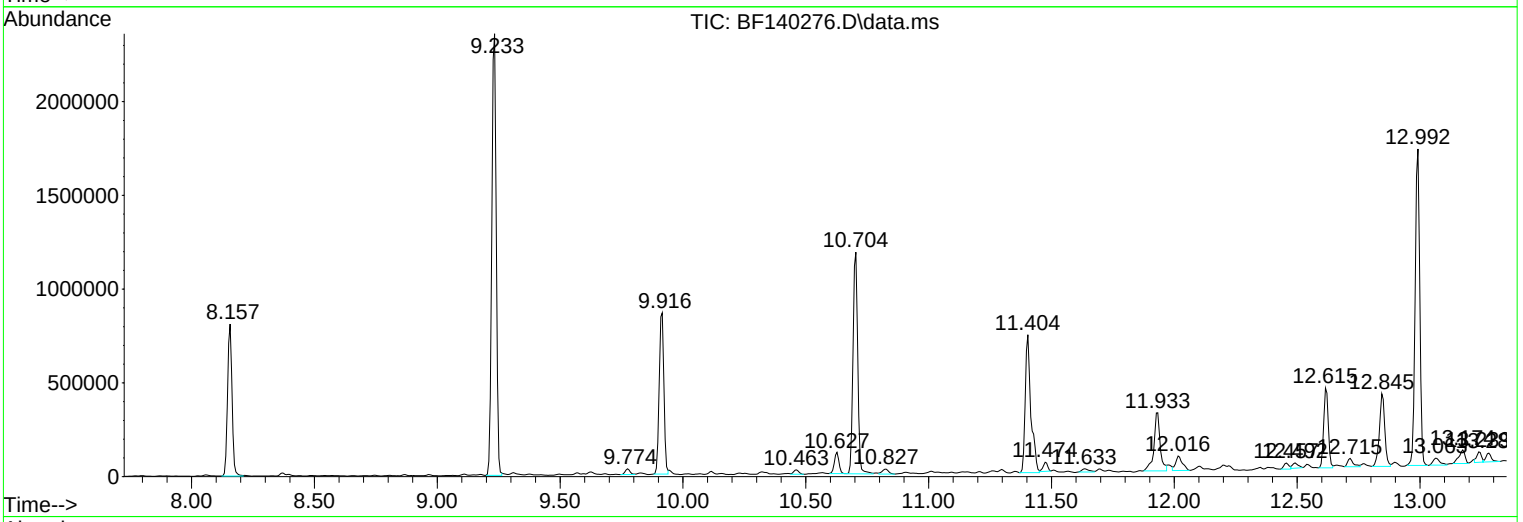
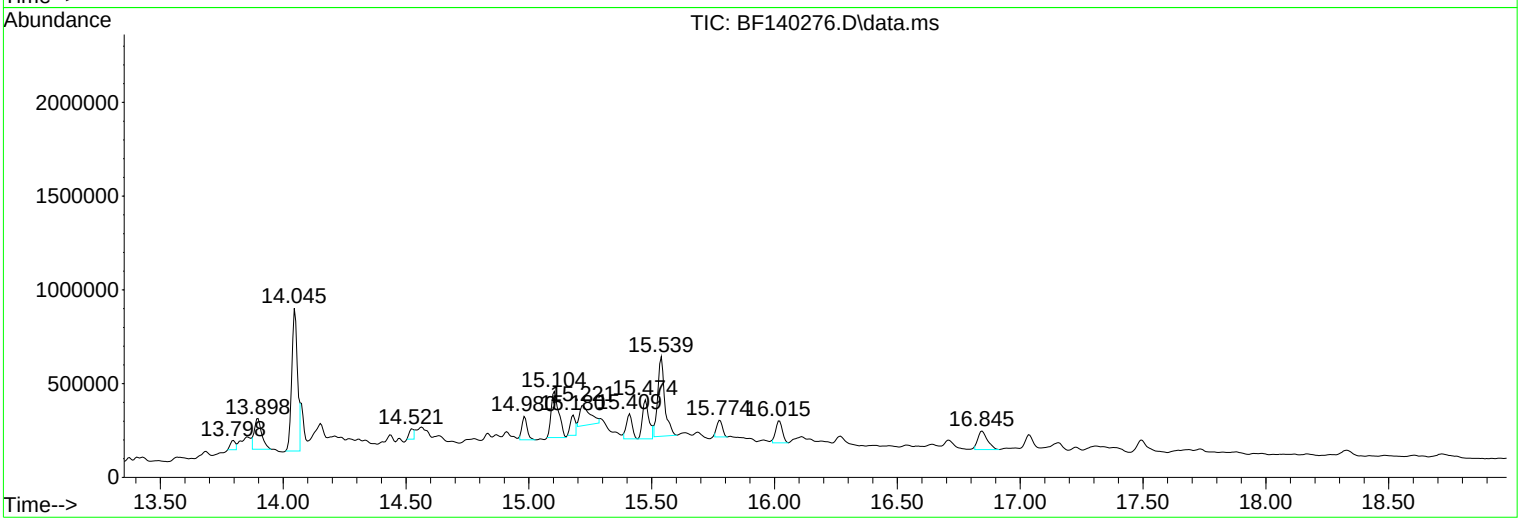
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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\BF110724\
Data File : BF140276.D
Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

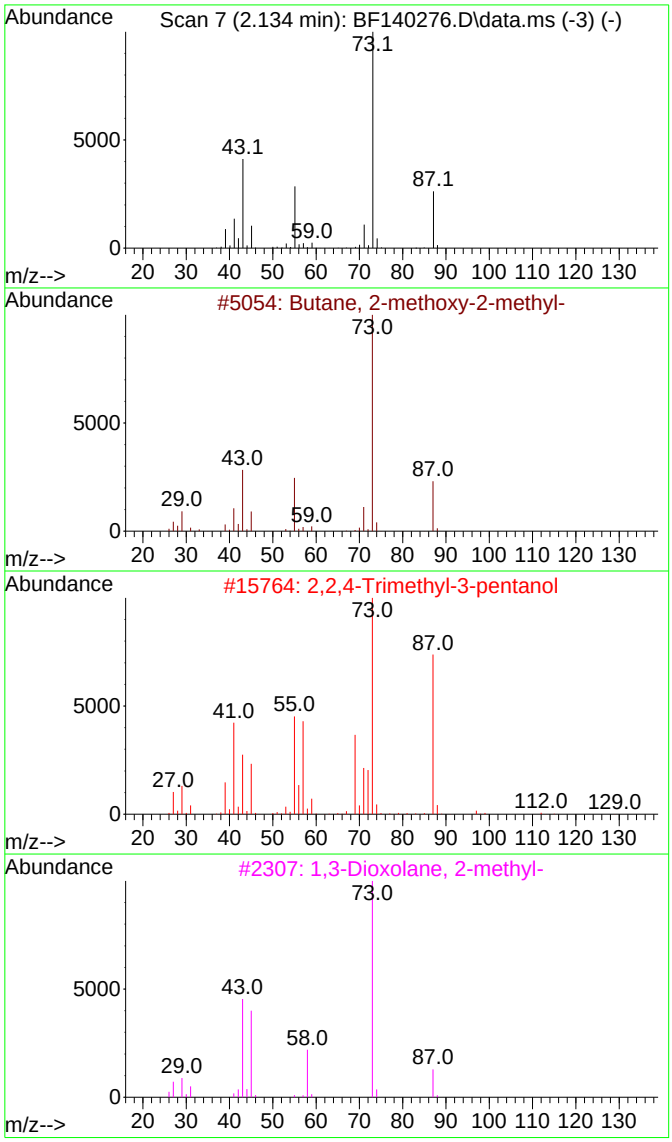
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

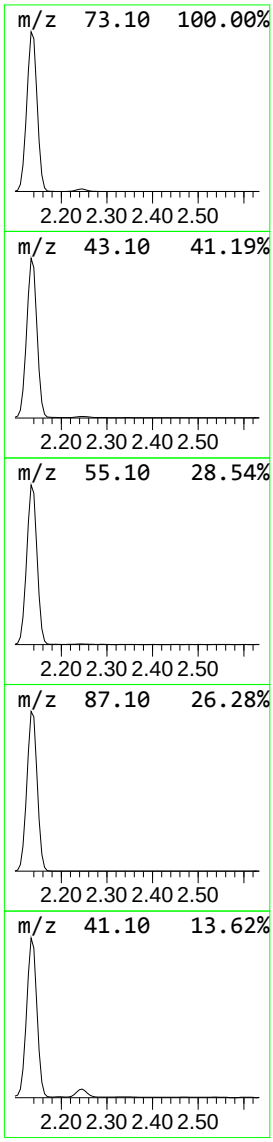
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	50.54 ng	2017830	1,4-Dichlorobenzene-d4	6.875

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF140276.D
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Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

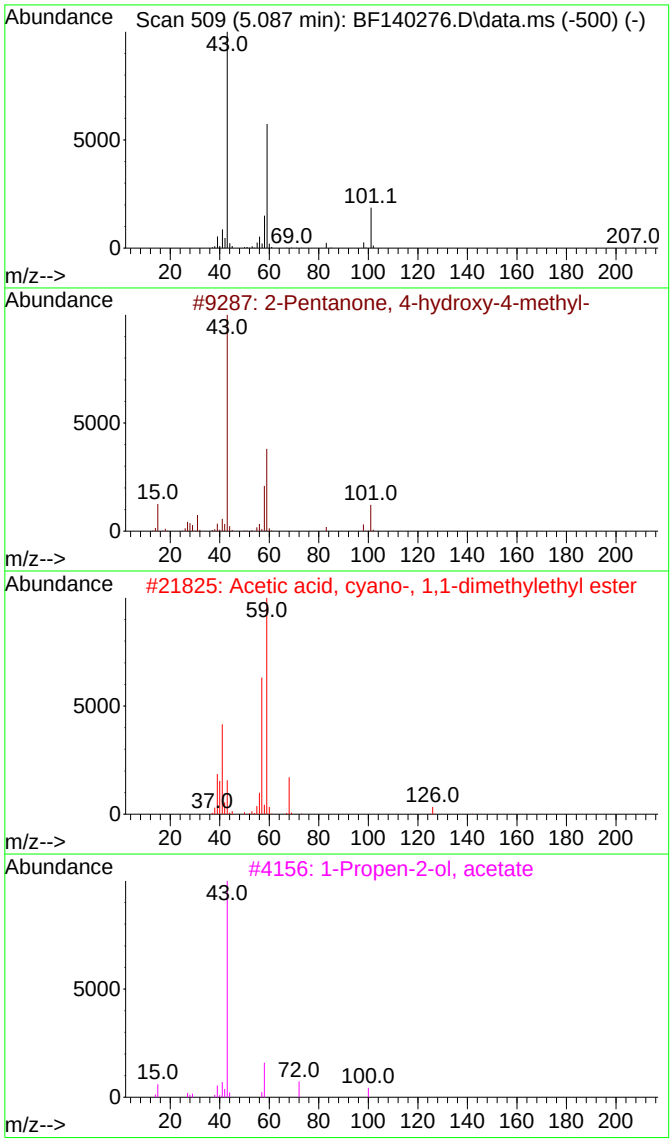
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

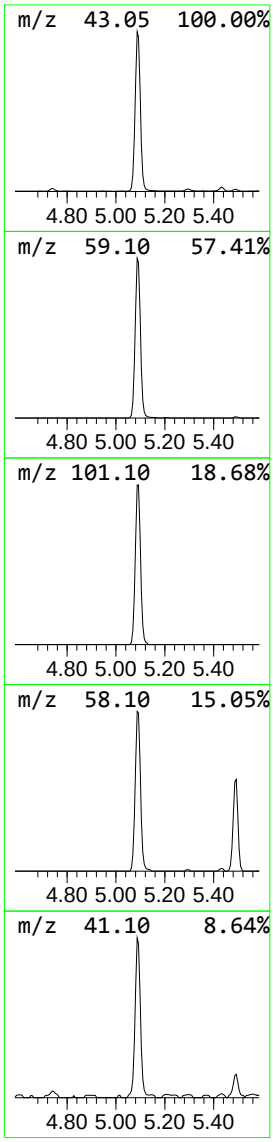
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	12.09 ng	482780	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140276.D
Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

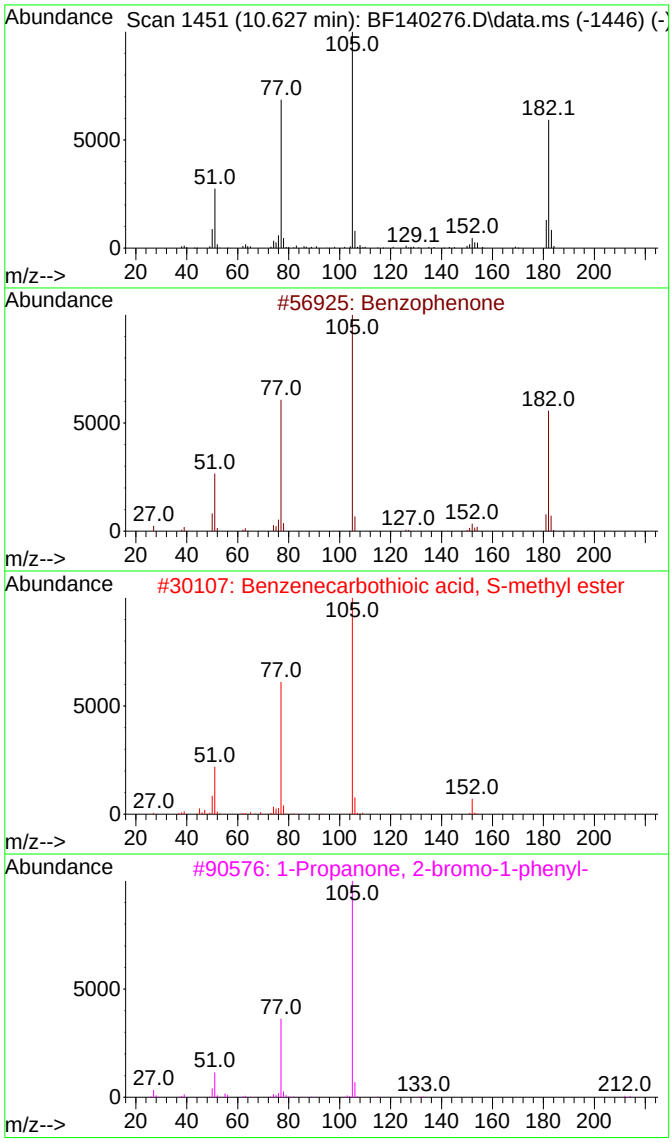
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

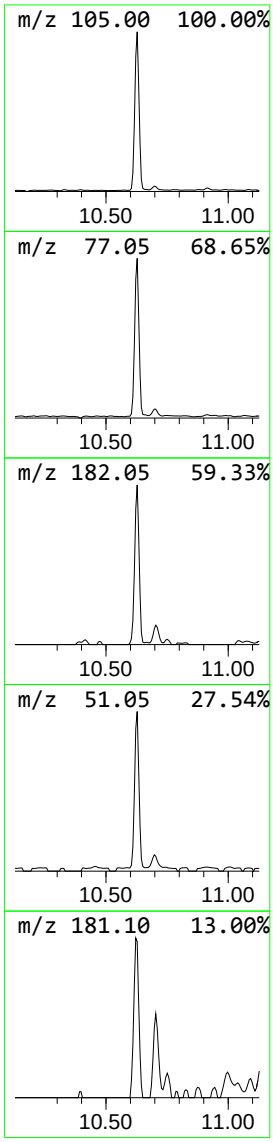
****

Peak Number 3 Benzophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.627	2.62 ng	146747	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	60
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47





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Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

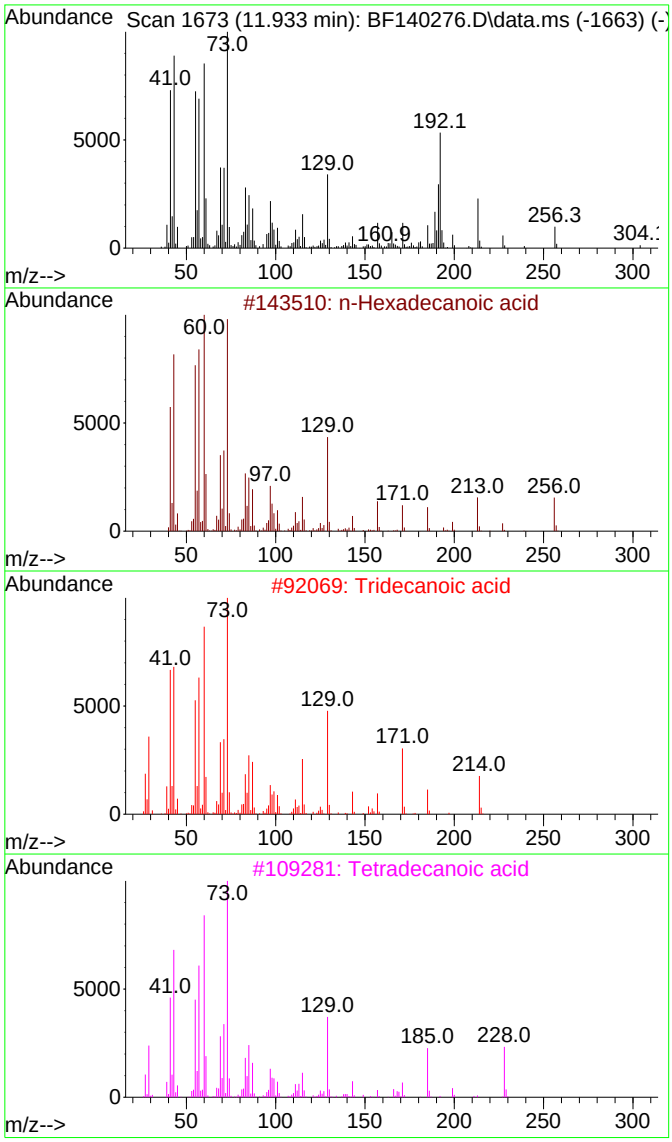
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

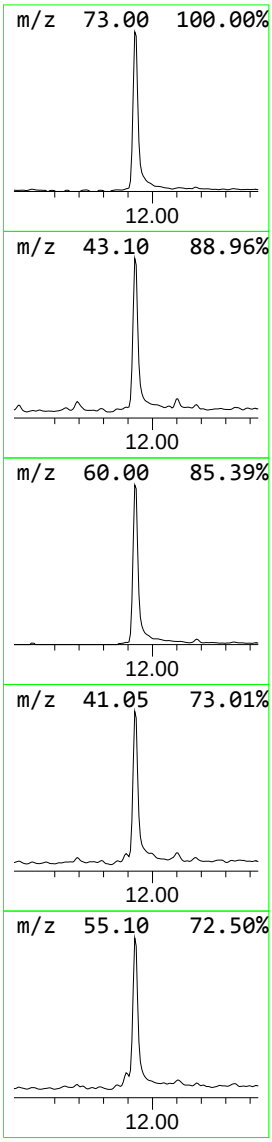
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	9.25 ng	545515	Phenanthrene-d10	11.404

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Data File : BF140276.D
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Sample : P4707-01
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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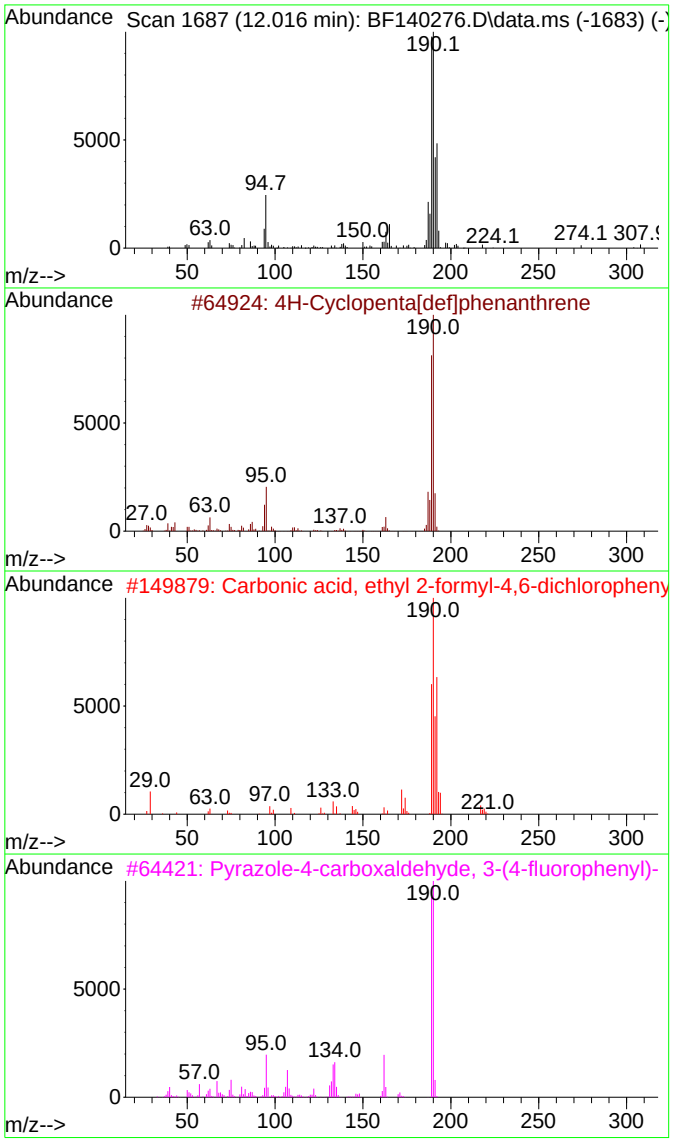
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

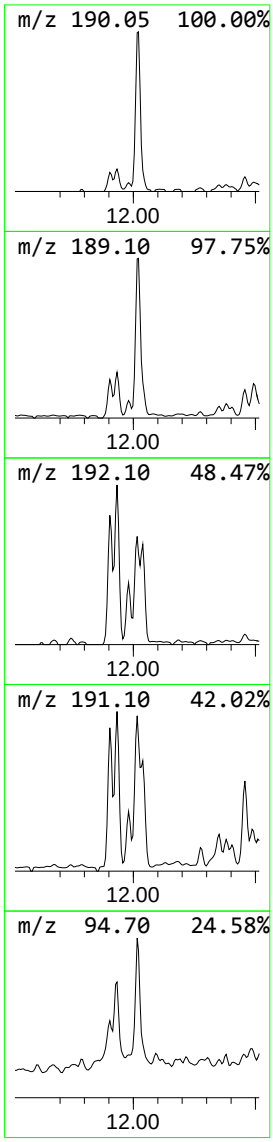
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	2.47 ng	145441	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	43
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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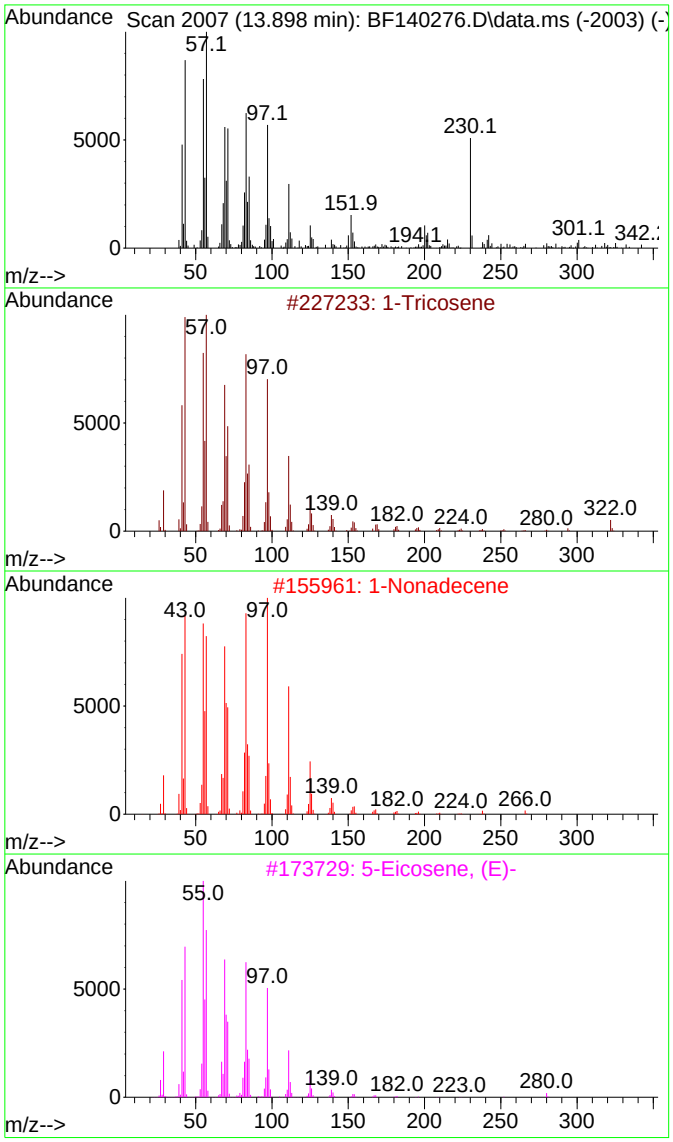
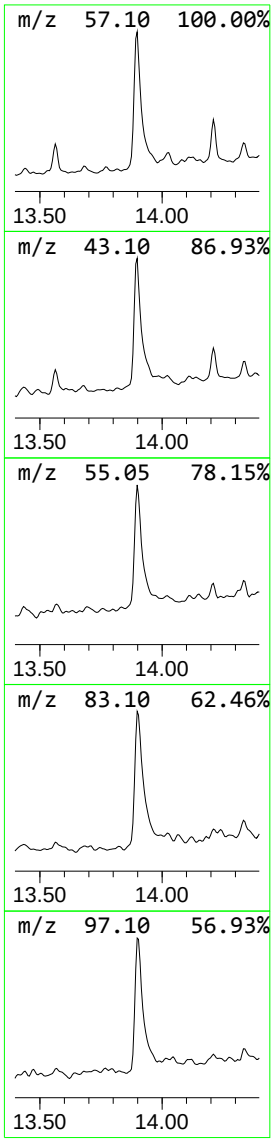
Peak Number 6 1-Tricosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.25 ng	335720	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	96
2	1-Nonadecene	266	C19H38	018435-45-5	95
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	86





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Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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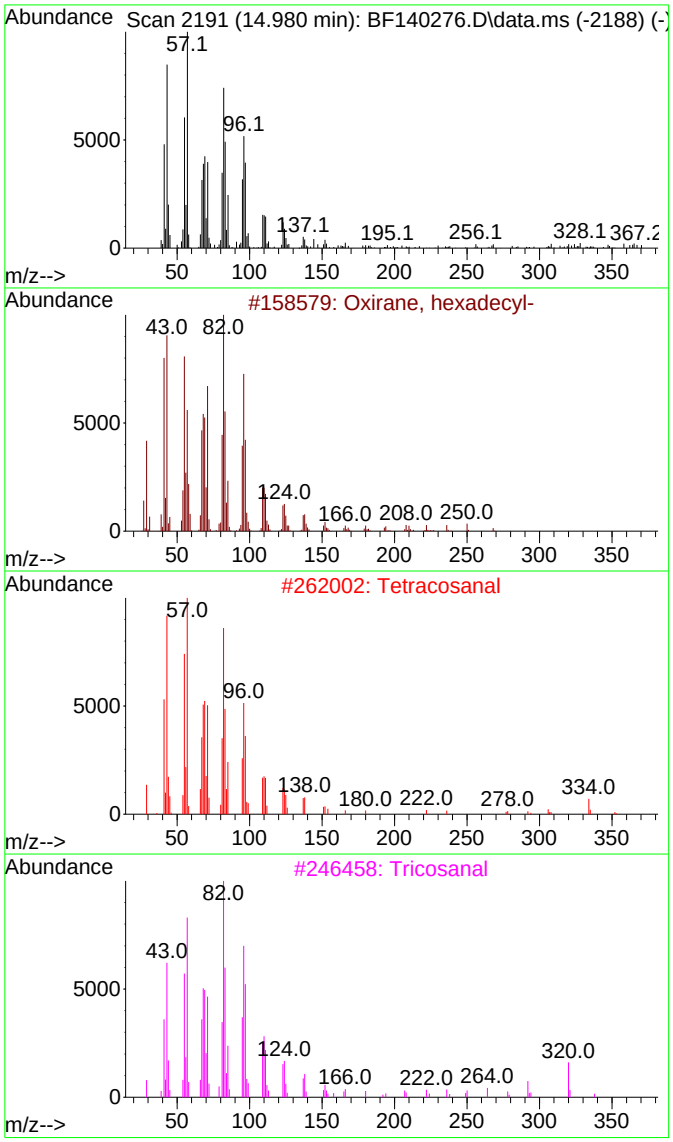
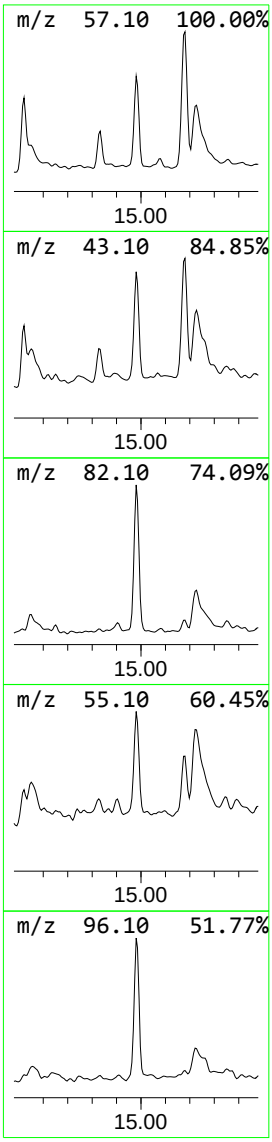
Peak Number 7 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	4.48 ng	182051	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2	Tetracosanal	352	C24H48O	057866-08-7	94
3	Tricosanal	338	C23H46O	072934-02-2	91
4	Eicosanal-	296	C20H40O	002400-66-0	90
5	Octadecanal	268	C18H36O	000638-66-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140276.D
Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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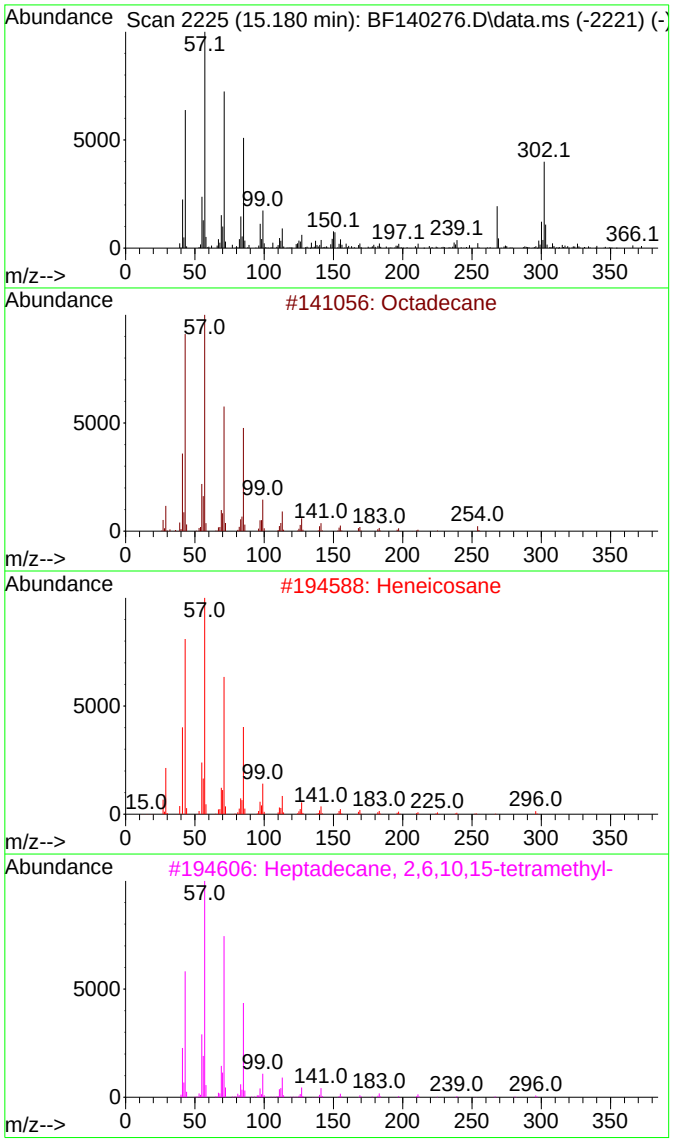
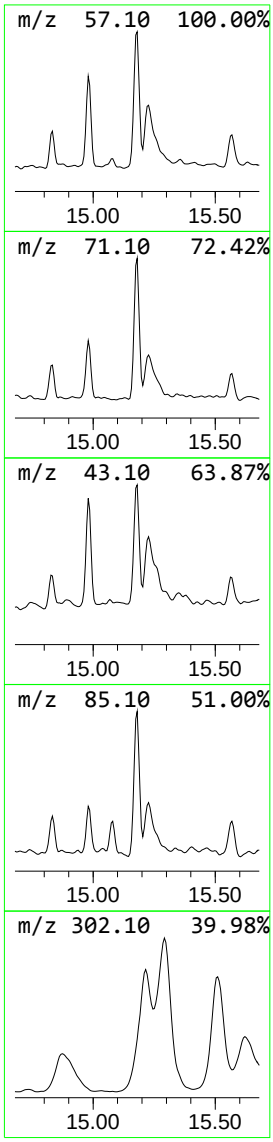
Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	3.85 ng	156510	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Heneicosane	296	C21H44	000629-94-7	80
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
4	Hexacosane	366	C26H54	000630-01-3	50
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	45





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Acq On : 07 Nov 2024 15:46
Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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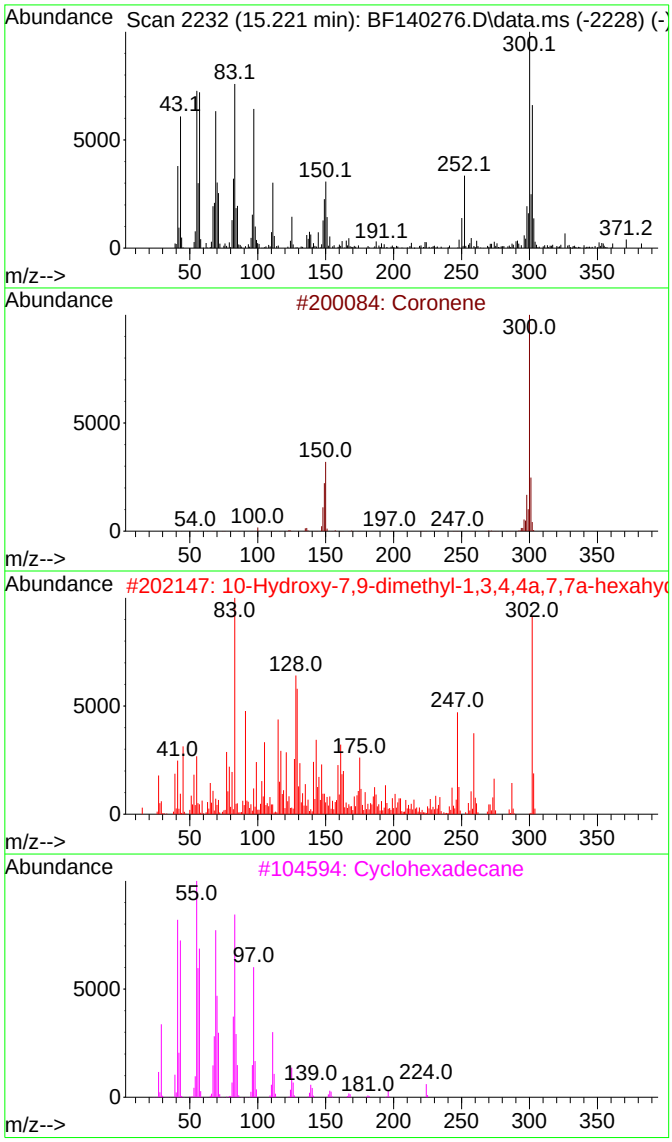
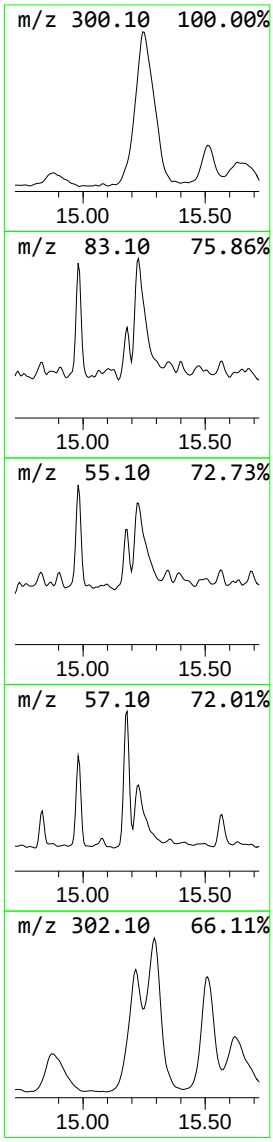
Peak Number 9 Coronene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	7.96 ng	323904	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Coronene	300	C24H12	000191-07-1	87
2	10-Hydroxy-7,9-dimethyl-1,3,4,4a...	302	C18H22O4	1000503-17-0	38
3	Cyclohexadecane	224	C16H32	000295-65-8	38
4	17-Pentatriacontene	491	C35H70	006971-40-0	30
5	Fumaric acid, 2-chloroethyl hexa...	402	C22H39ClO4	1000330-62-2	30





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Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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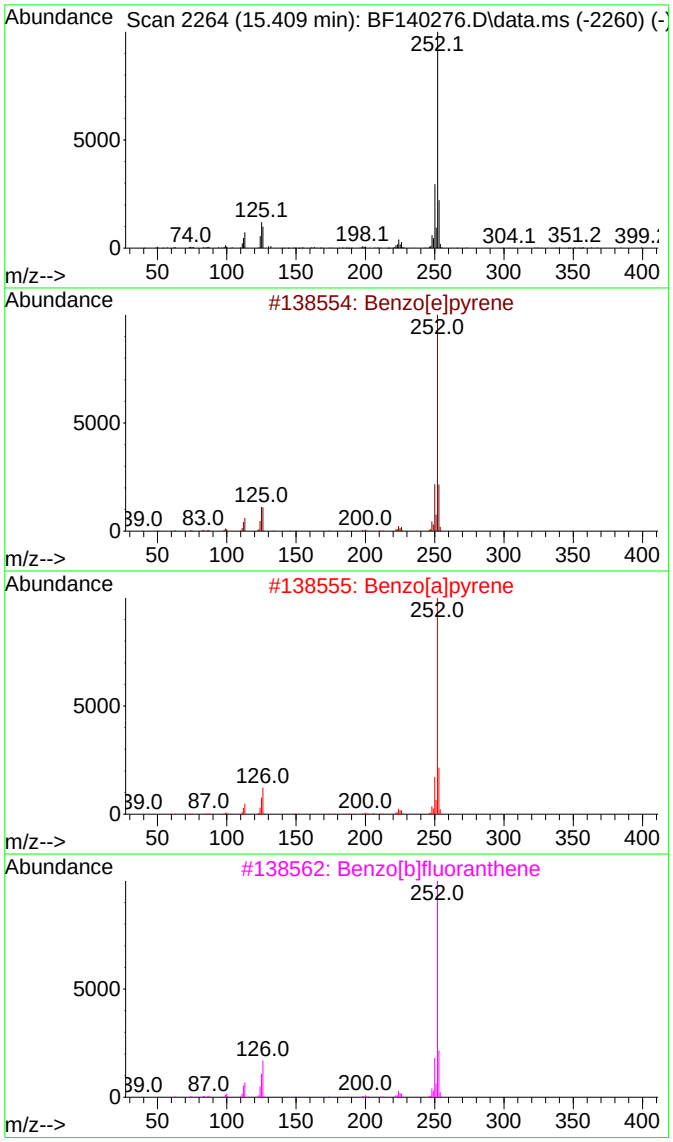
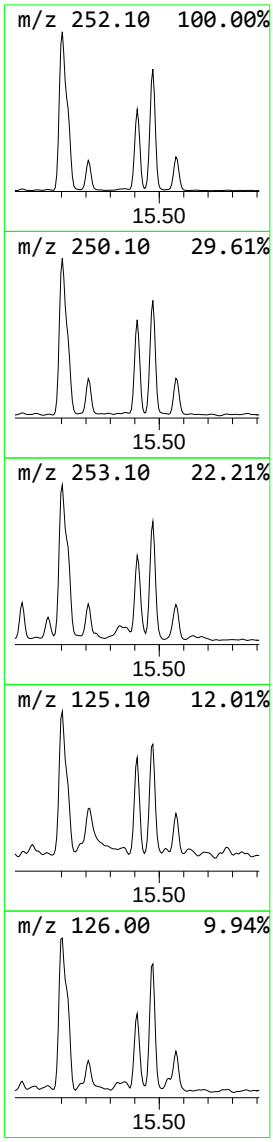
Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.409	5.27 ng	214493	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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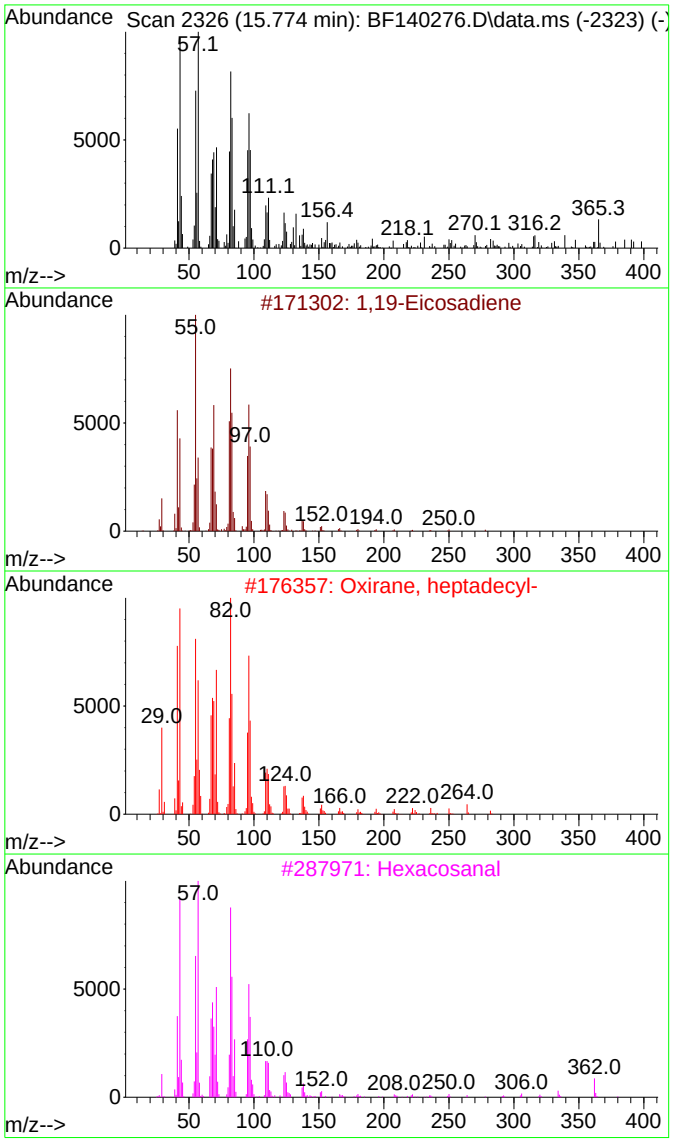
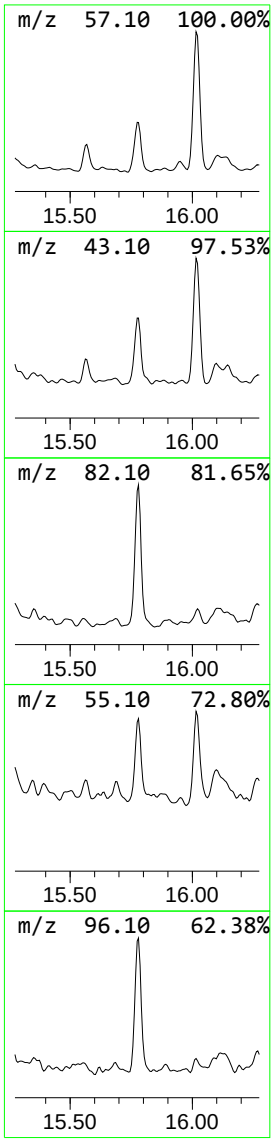
Peak Number 11 1,19-Eicosadiene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	3.44 ng	139988	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	94
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
3	Hexacosanal	380	C26H52O	026627-85-0	83
4	Octadecanal	268	C18H36O	000638-66-4	83
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81





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Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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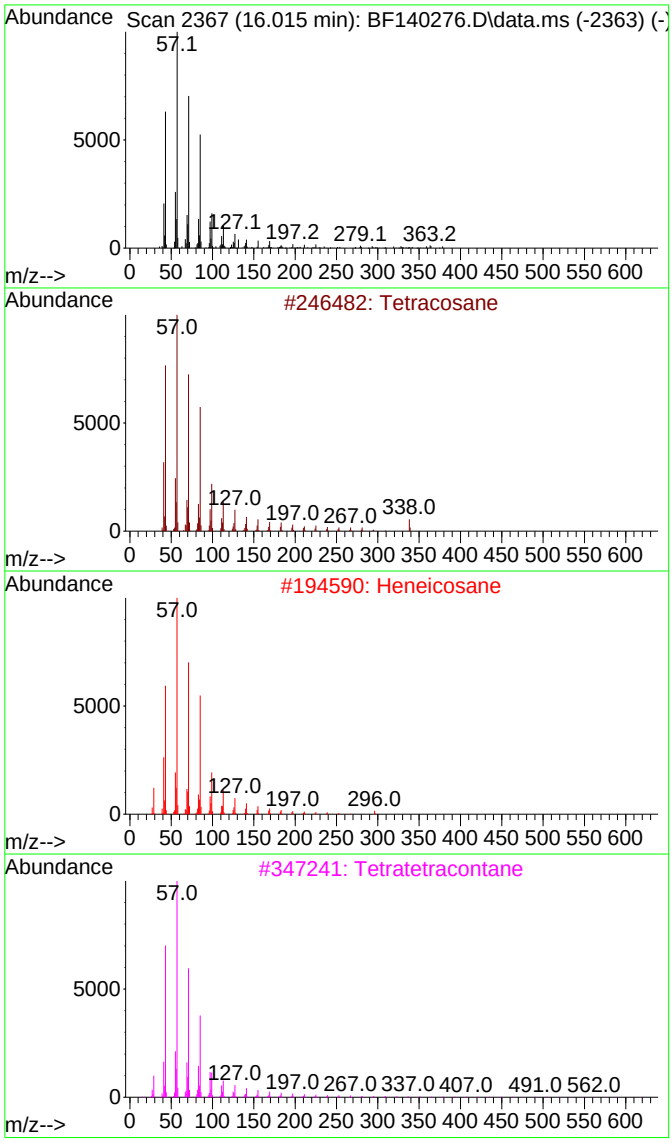
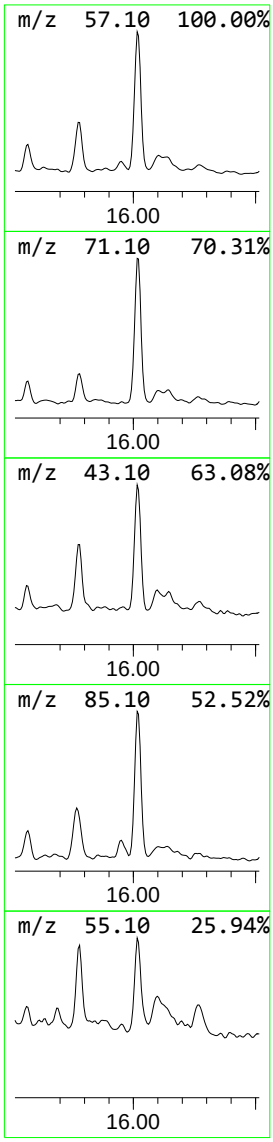
Peak Number 12 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	5.36 ng	218033	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Operator : RC/JU
Sample : P4707-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-110424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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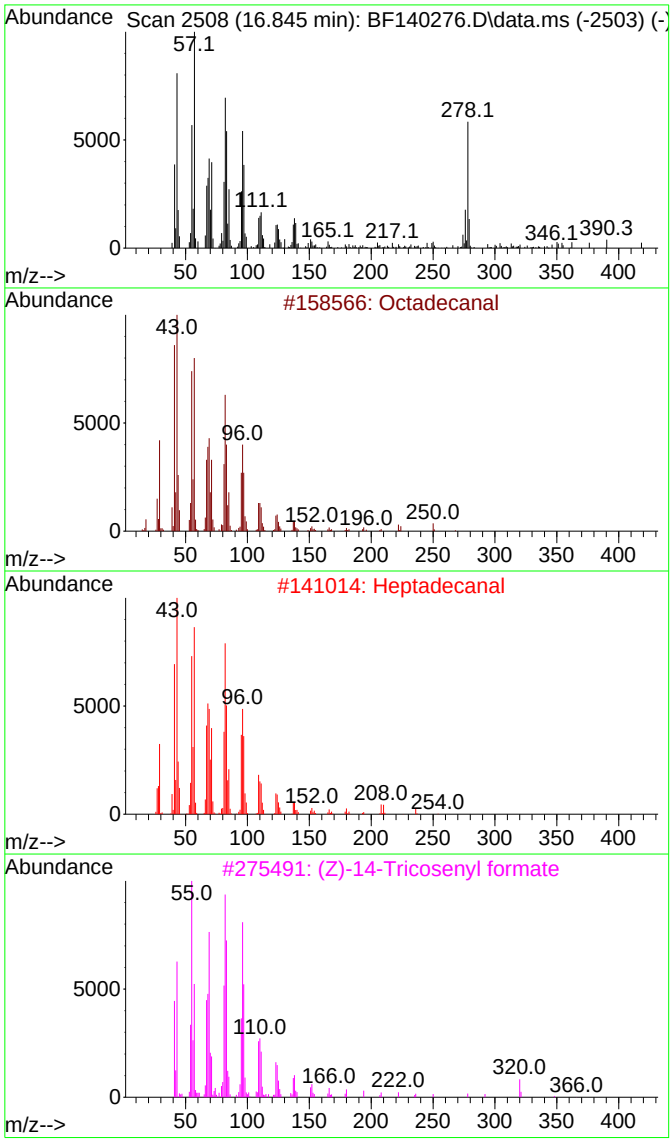
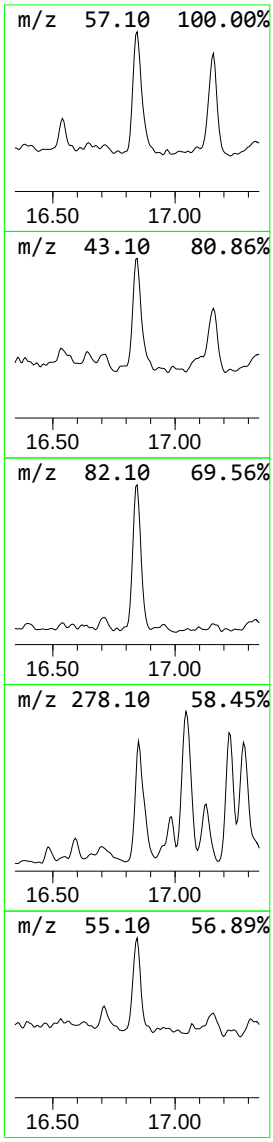
Peak Number 13 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.845	6.35 ng	258430	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	99
2	Heptadecanal	254	C17H34O	1000376-70-0	86
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	78
4	Tetracosanal	352	C24H48O	057866-08-7	74
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	70





Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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...	2.134	50.5	ng	2017830	1	6.875	798586	20.0
2-Pentanone, 4-...	5.087	12.1	ng	482780	1	6.875	798586	20.0
Benzophenone	10.627	2.6	ng	146747	3	9.916	1118300	20.0
n-Hexadecanoic ...	11.933	9.3	ng	545515	4	11.404	1179710	20.0
4H-Cyclopenta[d...	12.015	2.5	ng	145441	4	11.404	1179710	20.0
1-Tricosene	13.898	5.3	ng	335720	5	14.051	1279690	20.0
Oxirane, hexade...	14.980	4.5	ng	182051	6	15.539	813581	20.0
Octadecane	15.180	3.9	ng	156510	6	15.539	813581	20.0
Coronene	15.221	8.0	ng	323904	6	15.539	813581	20.0
Benzo[e]pyrene	15.409	5.3	ng	214493	6	15.539	813581	20.0
1,19-Eicosadiene	15.774	3.4	ng	139988	6	15.539	813581	20.0
Tetracosane	16.015	5.4	ng	218033	6	15.539	813581	20.0
Octadecanal	16.845	6.3	ng	258430	6	15.539	813581	20.0