LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	22	rVB	2600471	3193770	56.86%	6.542%
2	3.393	219	222	236	rBV	50615	104187	1.85%	0.213%
3	5.104	510	513	520	rVB	278715	306637	5.46%	0.628%
4	5.504	576	581	584	rBV	4567929	4697400	83.62%	9.622%
5	5.828	631	636	642	rBV	88385	75032	1.34%	0.154%
6	6.510	747	752	755	rBV	4306782	4654578	82.86%	9.534%
7	6.881	812	815	819	rVB	1901647	1698823	30.24%	3.480%
8	7.445	906	911	914	rBV	3498103	3034111	54.01%	6.215%
9	7.692	950	953	957	rBV	190416	163340	2.91%	0.335%
10	7.969	997	1000	1007	rVB	79936	68370	1.22%	0.140%
11	8.163	1029	1033	1036	rBV	2781732	2193969	39.06%	4.494%
12	8.475	1082	1086	1092	rBV	192396	194510	3.46%	0.398%
13	9.239	1212	1216	1219	rBV	6704392	5617224	100.00%	11.506%
14	9.669	1286	1289	1297	rBV	197827	196768	3.50%	0.403%
15	9.916	1328	1331	1335	rBV	2468478	2202291	39.21%	4.511%
16	10.016	1343	1348	1351	rVB2	67581	79925	1.42%	0.164%
17	10.704	1461	1465	1476	rBV	3126749	2703132	48.12%	5.537%
18	10.886	1493	1496	1498	rBV	116980	105854	1.88%	0.217%
19	10.921	1498	1502	1505	rVV2	95628	123812	2.20%	0.254%
20	10.951	1505	1507	1509	rVV2	98803	75366	1.34%	0.154%
21	11.063	1523	1526	1530	rBV3	94371	105050	1.87%	0.215%
22	11.104	1530	1533	1535	rBV	95870	86204	1.53%	0.177%
23	11.404	1578	1584	1586	rBV	2110151	1732233	30.84%	3.548%
24	11.427	1586	1588	1591	rVB	230754	174065	3.10%	0.357%
25	11.904	1664	1669	1670	rBV3	54713	78102	1.39%	0.160%
26	11.927	1670	1673	1685	rVB2	620899	604964	10.77%	1.239%
27	12.615	1786	1790	1792	rBV	589752	508028	9.04%	1.041%
28	12.651	1794	1796	1803	rVB7	49027	72890	1.30%	0.149%
29	12.710	1803	1806	1809	rBV	136578	130389	2.32%	0.267%
30	12.839	1824	1828	1831	rVV	423783	399749	7.12%	0.819%
31	12.868	1831	1833	1841	rVB2	86723	142992	2.55%	0.293%
32	12.986	1849	1853	1857	rVB	4773101	3949637	70.31%	8.090%
33	13.215	1888	1892	1894	rBV	59018	67173	1.20%	0.138%
34	13.557	1946	1950	1959	rVB4	36418	83839	1.49%	0.172%
35	13.786	1985	1989	1992	rBV2	48613	70554	1.26%	0.145%
36	13.886	2003	2006	2017	rBV2	295393	460871	8.20%	0.944%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.039	2024	2032	2035	rBV	2024111	2016935	35.91%	4.131%
38	14.062	2035	2036	2044	rVB	333809	245169	4.36%	0.502%
39	14.509	2109	2112	2117	rBV3	189883	298321	5.31%	0.611%
40	14.821	2162	2165	2168	rBV	62756	66786	1.19%	0.137%
41	14.898	2174	2178	2181	rBV2	108262	118211	2.10%	0.242%
42	14.968	2186	2190	2196	rBV	677328	680509	12.11%	1.394%
43	15.080	2205	2209	2212	rBV	278442	419530	7.47%	0.859%
44	15.162	2219	2223	2225	rBV	232403	241546	4.30%	0.495%
45	15.192	2225	2228	2249	rVB2	719584	1560649	27.78%	3.197%
46	15.386	2257	2261	2266	rVB	144193	185522	3.30%	0.380%
47	15.445	2267	2271	2277	rBV	200302	240659	4.28%	0.493%
48	15.509	2278	2282	2286	rBV	1060490	1294339	23.04%	2.651%
49	15.751	2319	2323	2329	rBV2	192268	259943	4.63%	0.532%
50	15.992	2359	2364	2369	rVB	189320	265325	4.72%	0.543%
51	16.068	2371	2377	2383	rBV6	100228	298532	5.31%	0.611%
52	16.803	2498	2502	2510	rVB4	105156	207969	3.70%	0.426%
53	16.980	2528	2532	2539	rBV2	63765	121311	2.16%	0.248%
54	17.180	2562	2566	2571	rVB6	43495	68297	1.22%	0.140%
55	17.427	2605	2608	2613	rVB	45655	75463	1.34%	0.155%

Sum of corrected areas: 48820855

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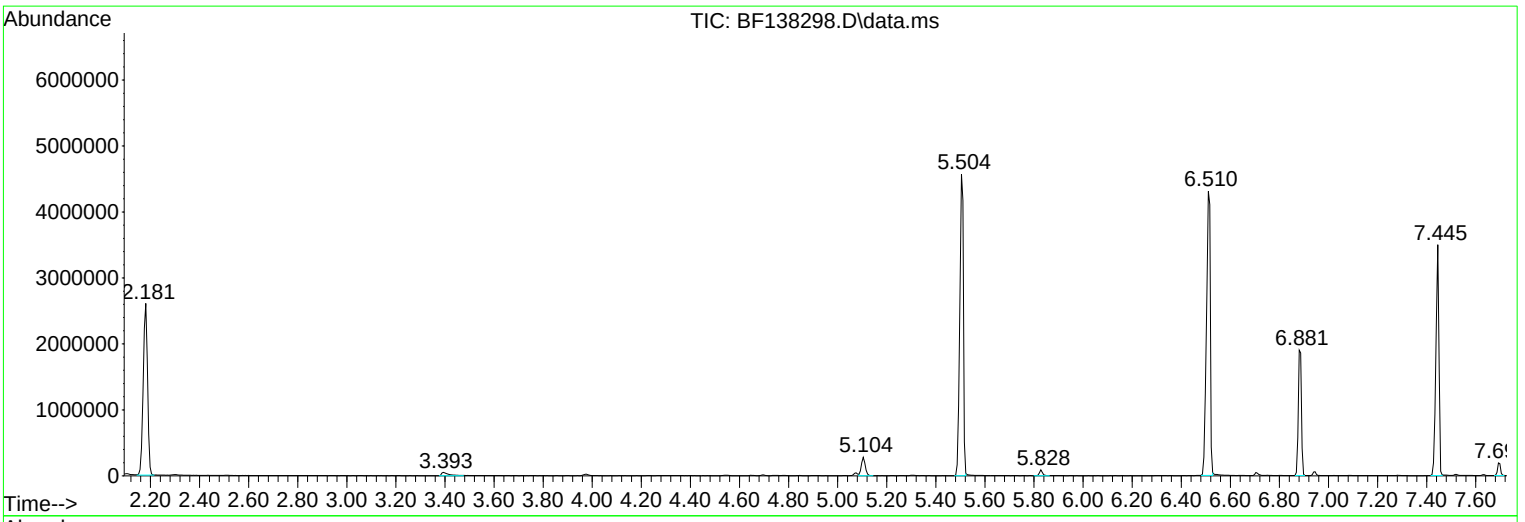
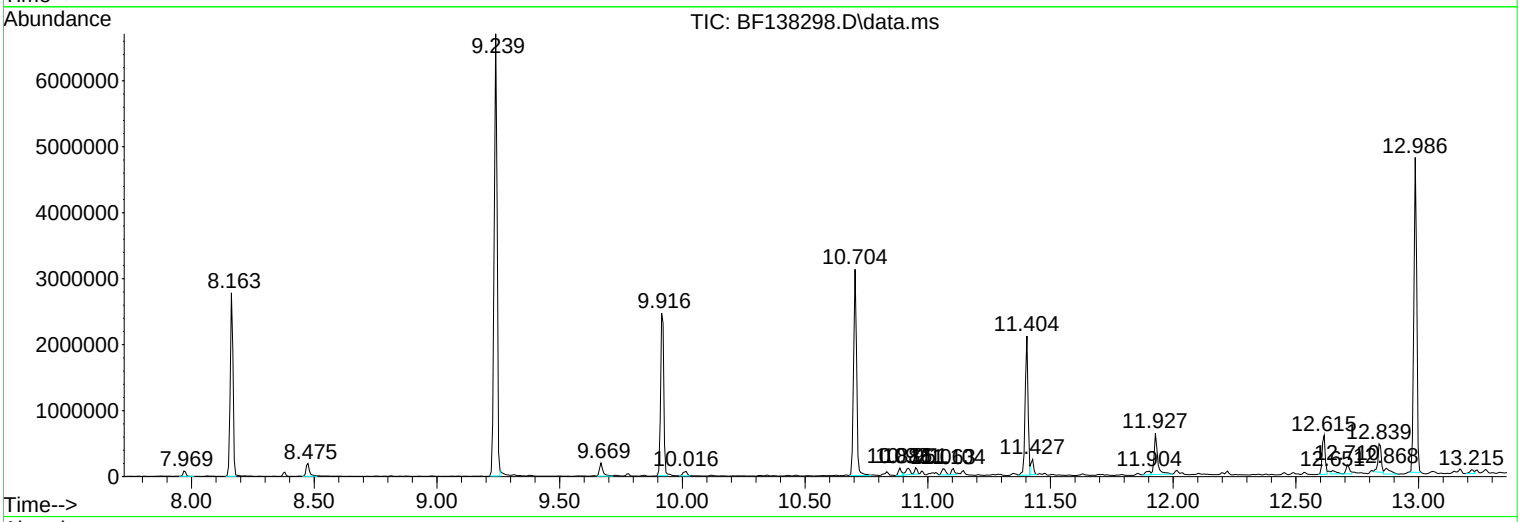
Misc :
ALS Vial : 22 Sample Multiplier: 1

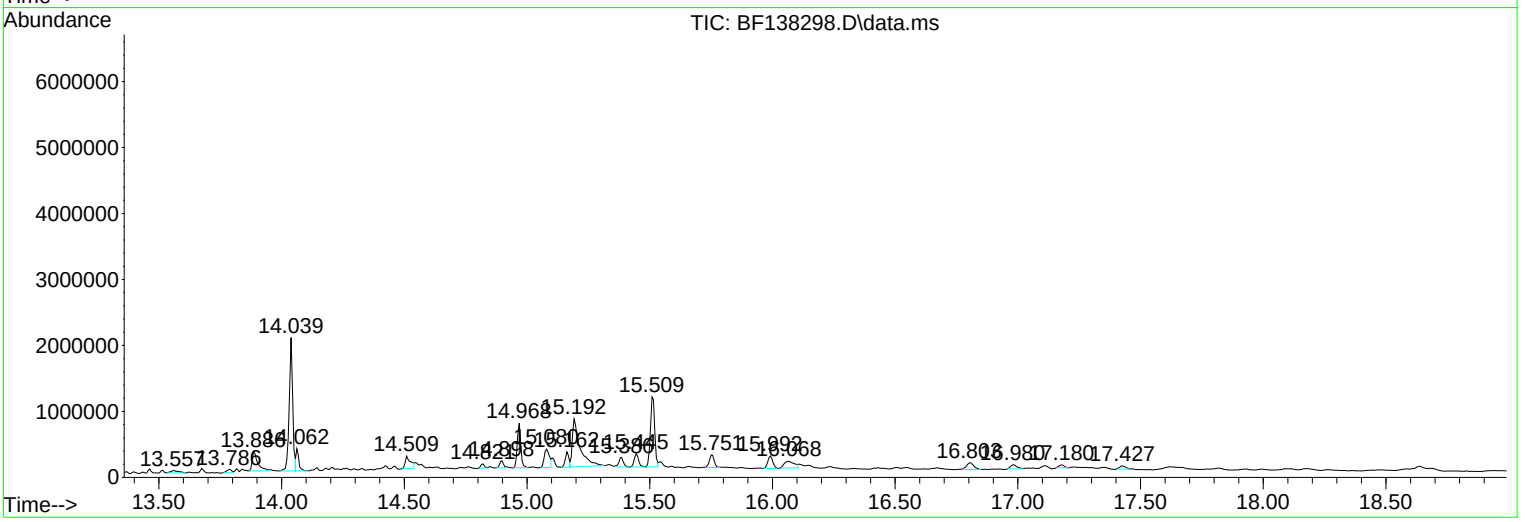
Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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 : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
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Instrument :
BNA_F
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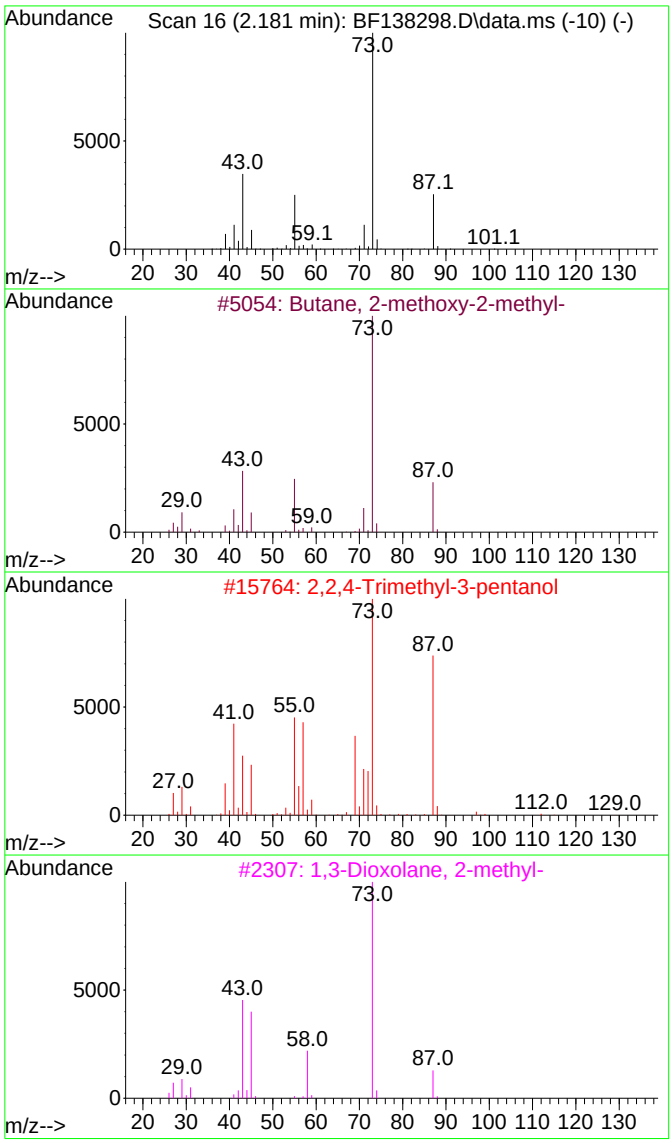
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

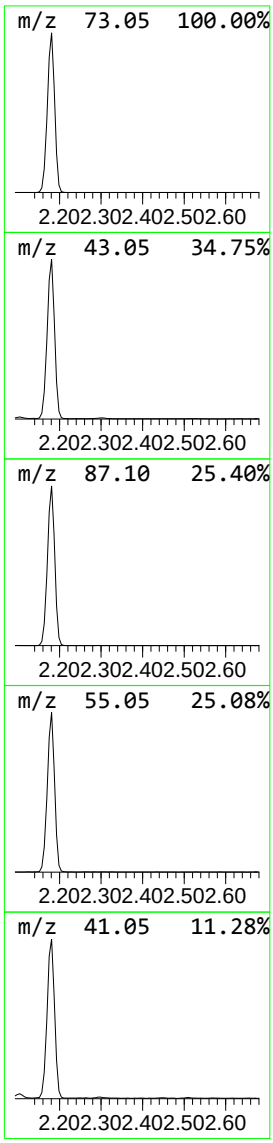
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	37.60 ng	3193770	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23





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Data File : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

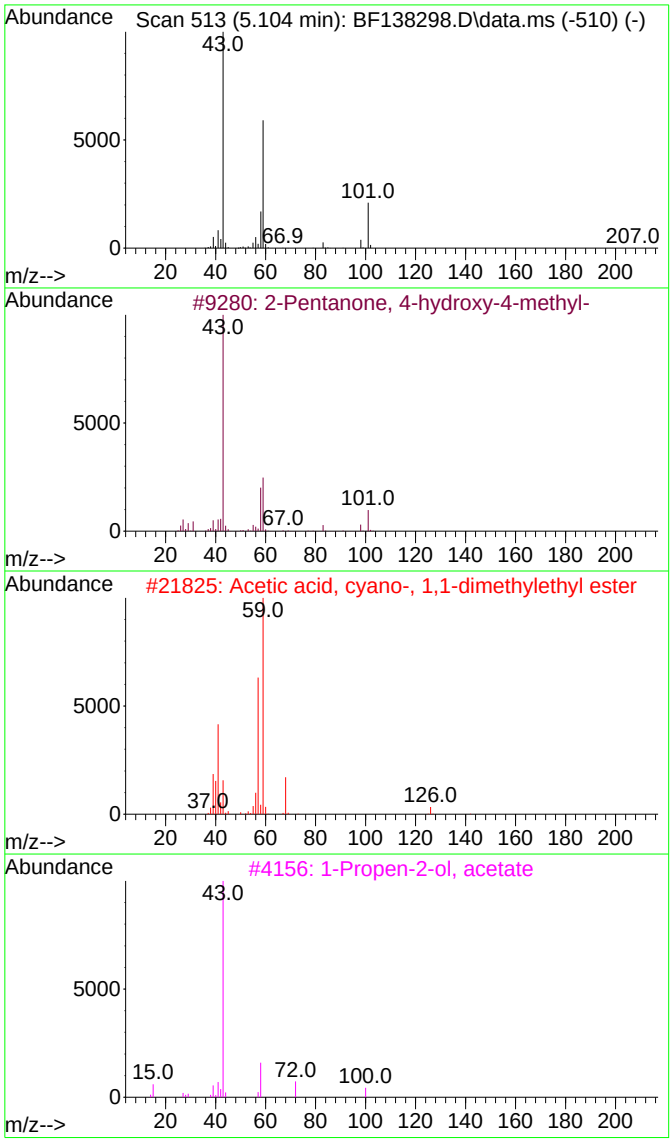
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

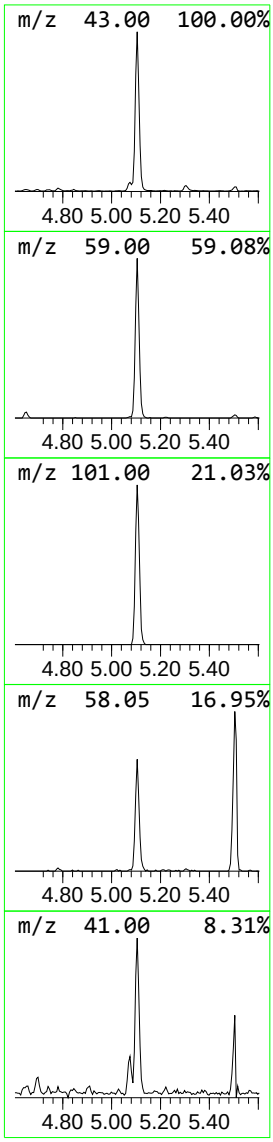
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.61 ng	306637	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
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Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

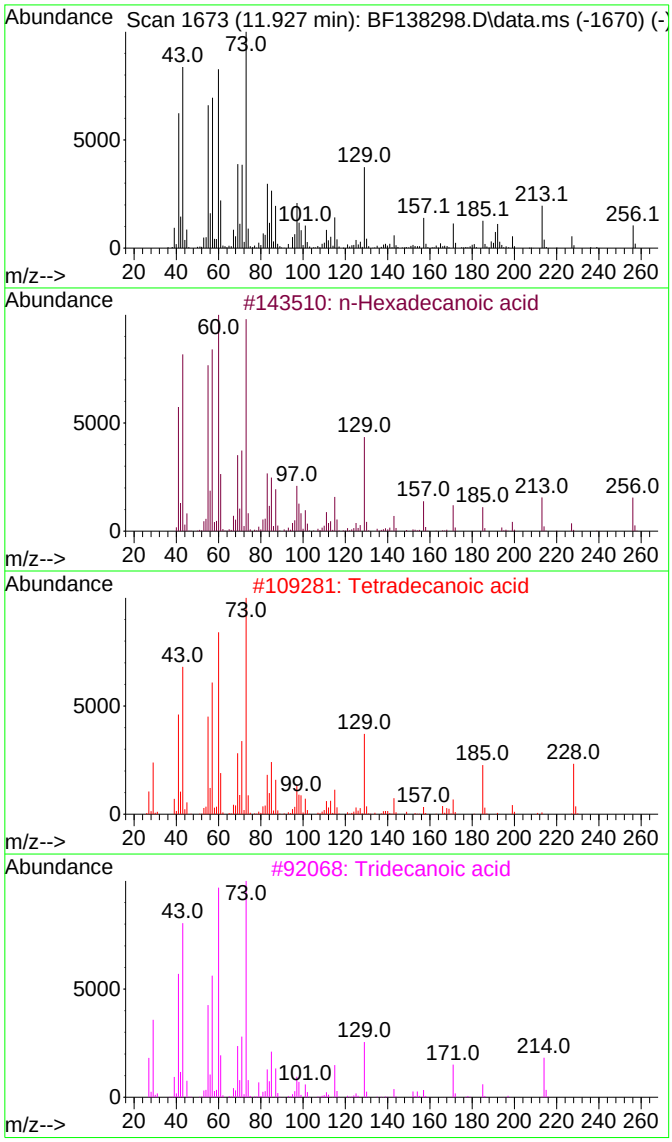
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

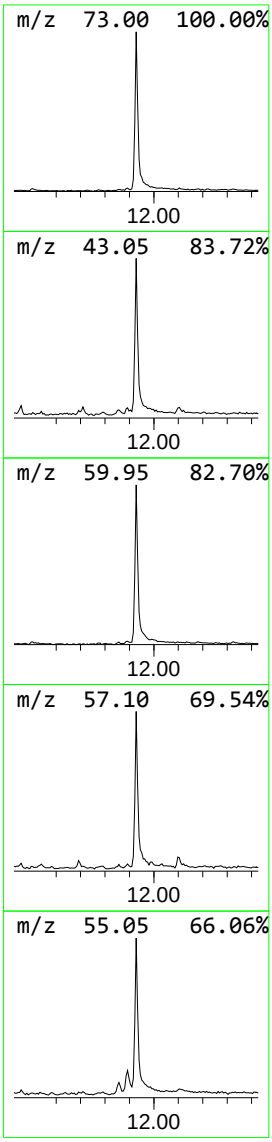
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	6.98 ng	604964	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
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Instrument :
BNA_F
ClientSampleId :
OSTL-B1

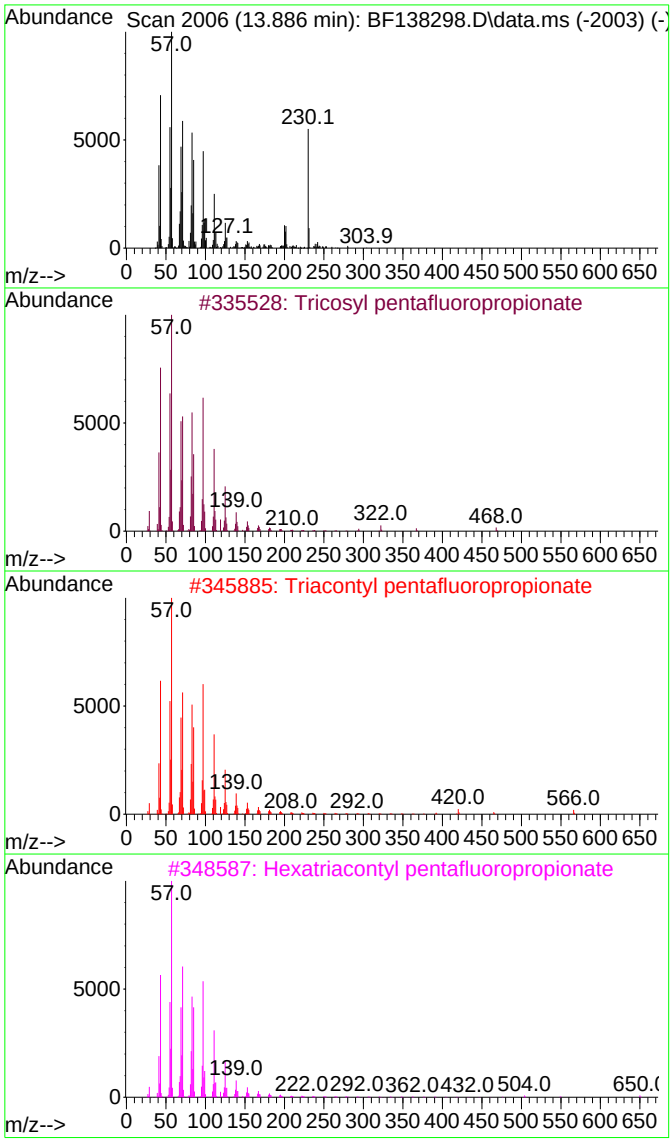
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

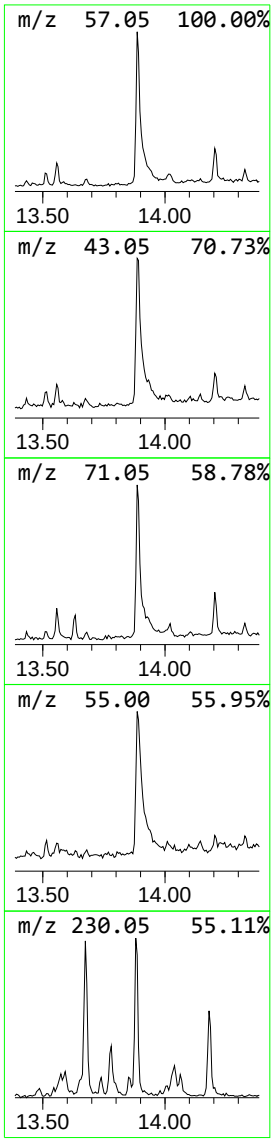
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Tricosyl pentafluoropropionate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.57 ng	460871	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	70
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	70
3	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	70
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	70
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	64





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Sample : P2977-07
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

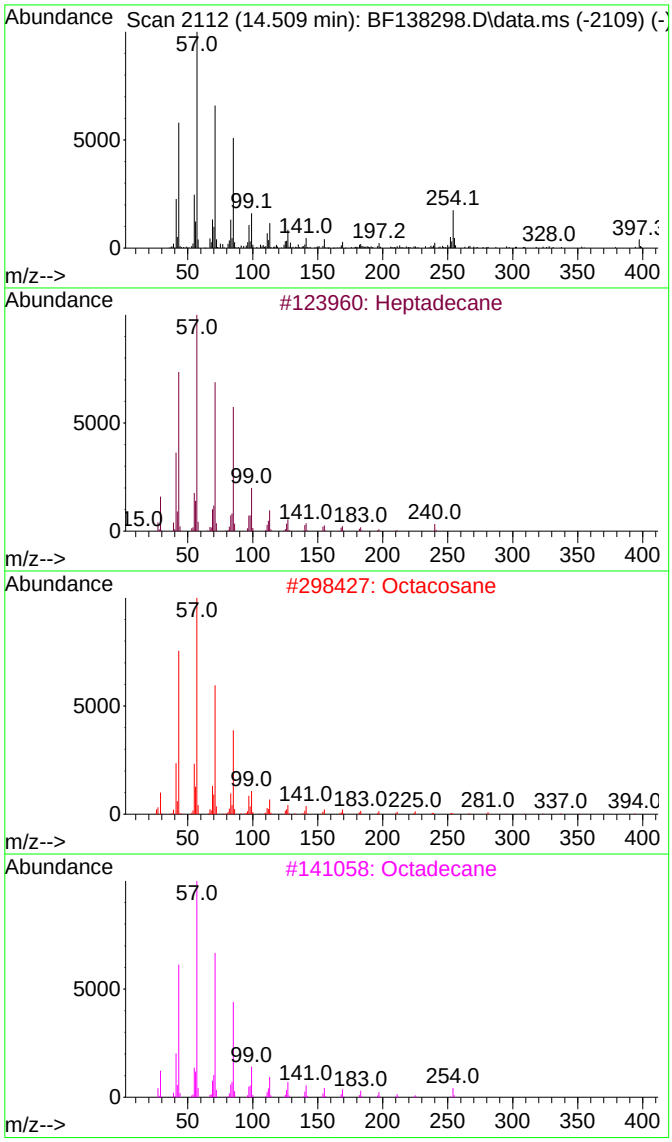
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

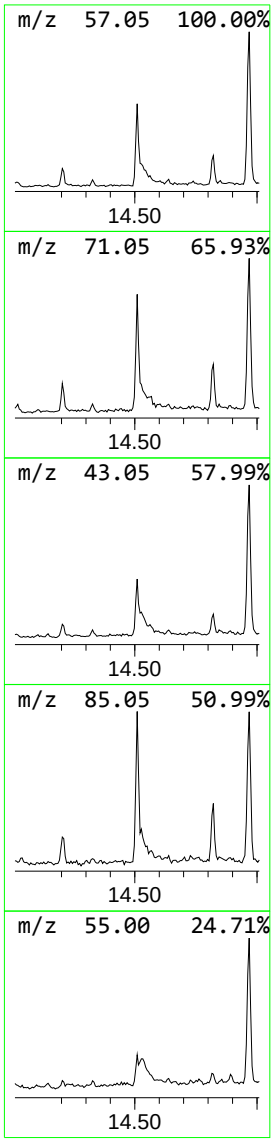
****

Peak Number 5 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.509	2.96 ng	298321	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Triacontane	422	C30H62	000638-68-6	87





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Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

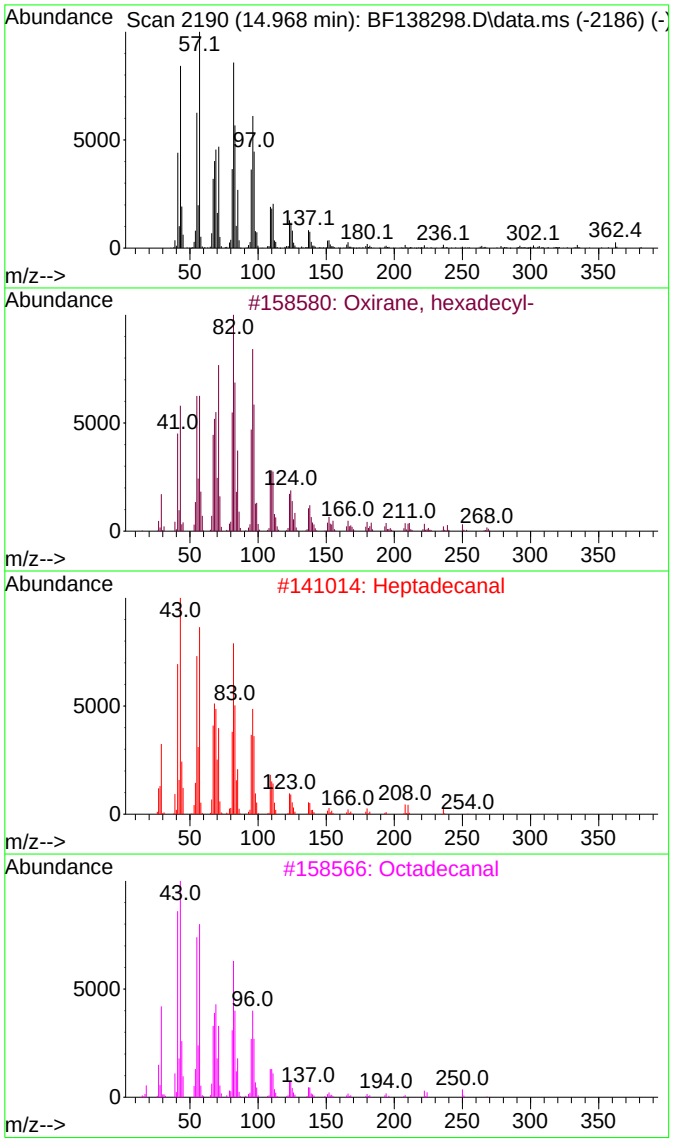
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

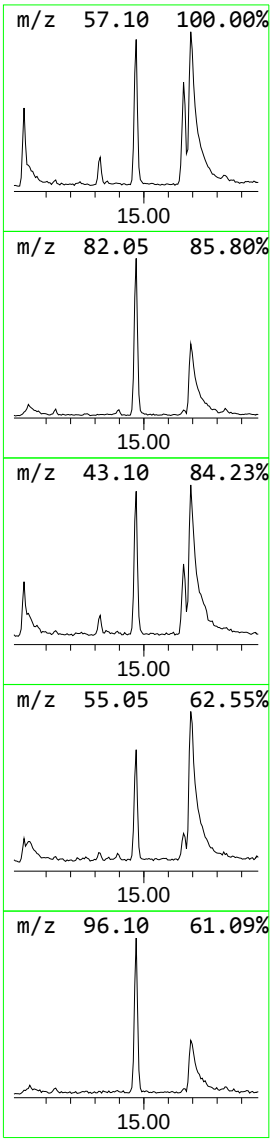
****

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	10.52 ng	680509	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	Heptadecanal	254	C17H34O	1000376-70-0	93
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5	1,19-Eicosadiene	278	C20H38	014811-95-1	90





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Data File : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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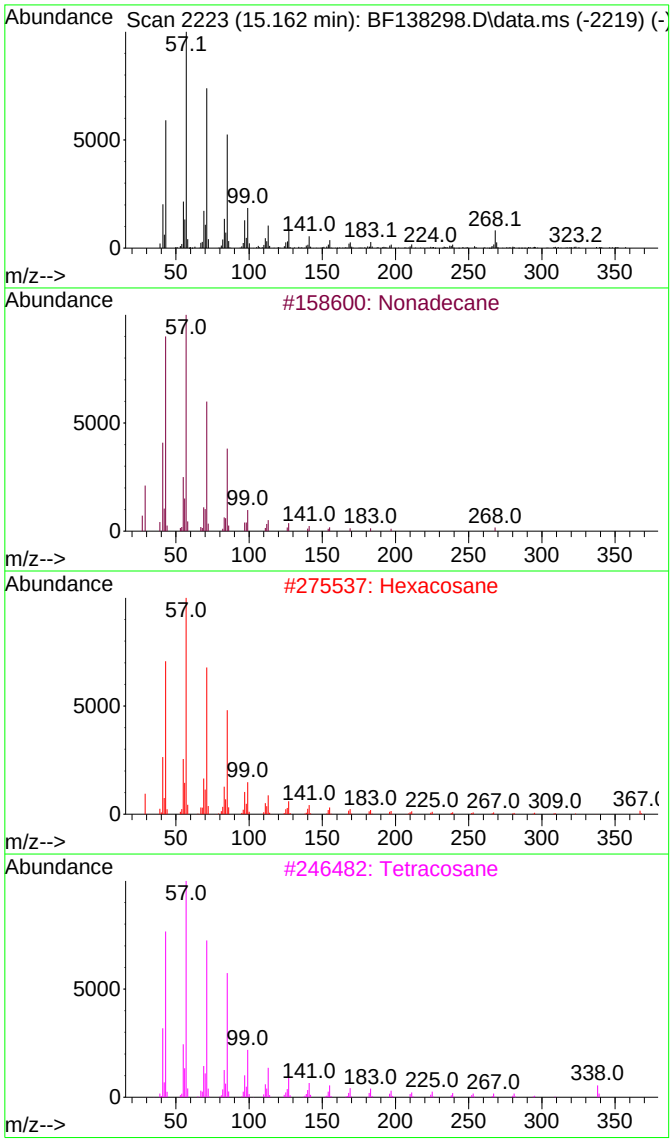
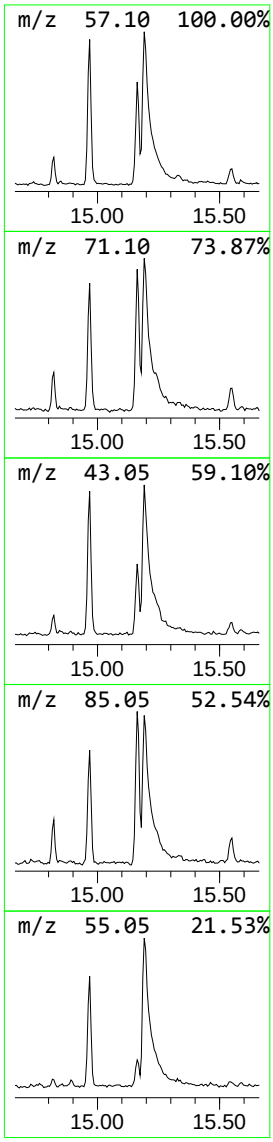
Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.162	3.73 ng	241546	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138298.D
Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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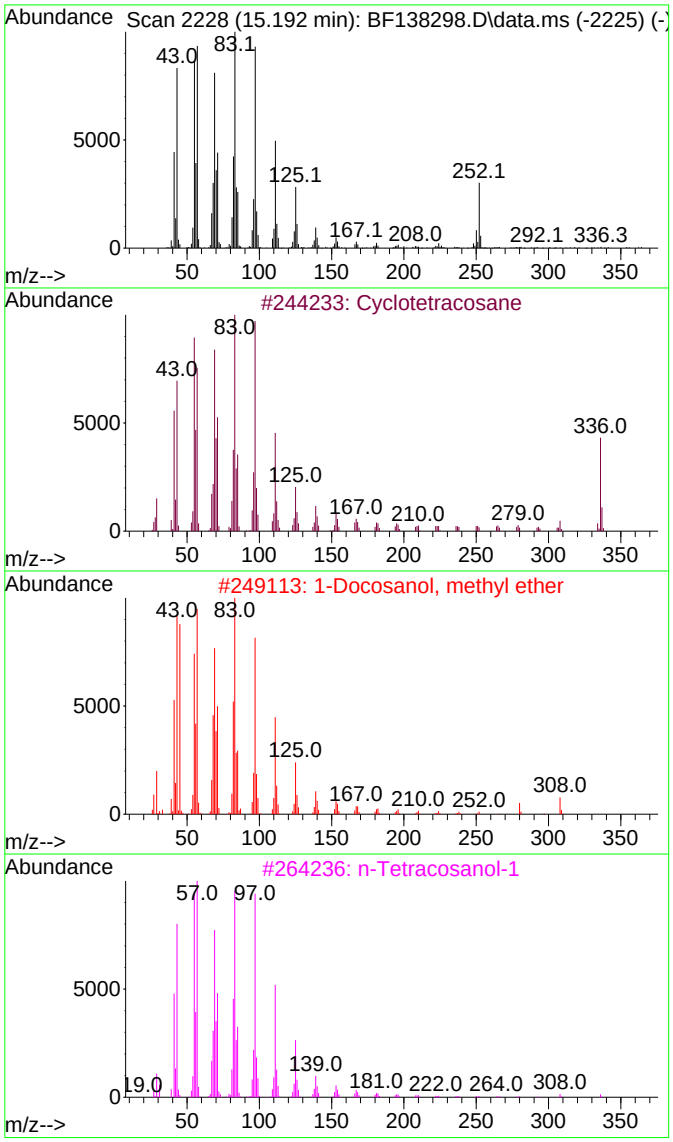
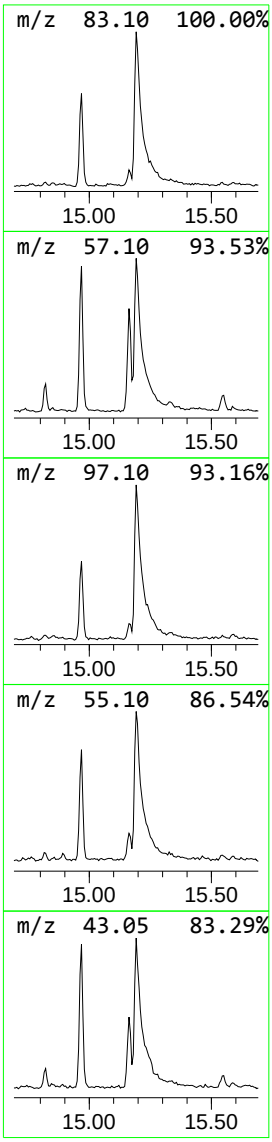
Peak Number 8 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	24.11 ng	1560650	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	98
2	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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Acq On : 21 Jun 2024 21:38
Operator : CG\JU
Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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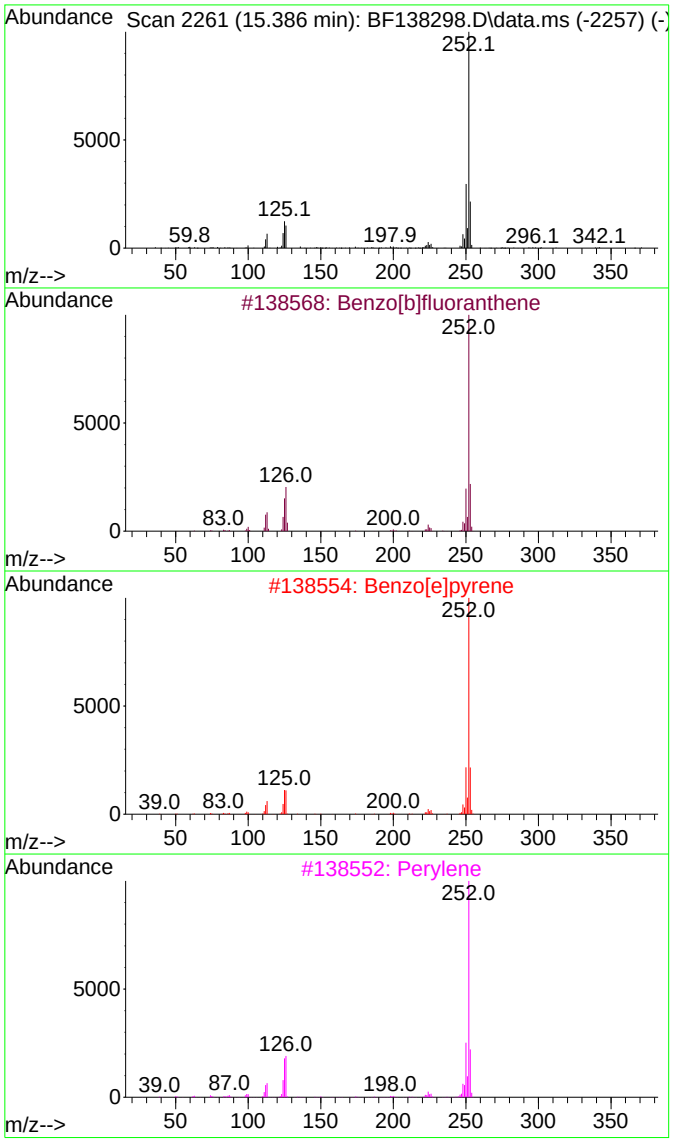
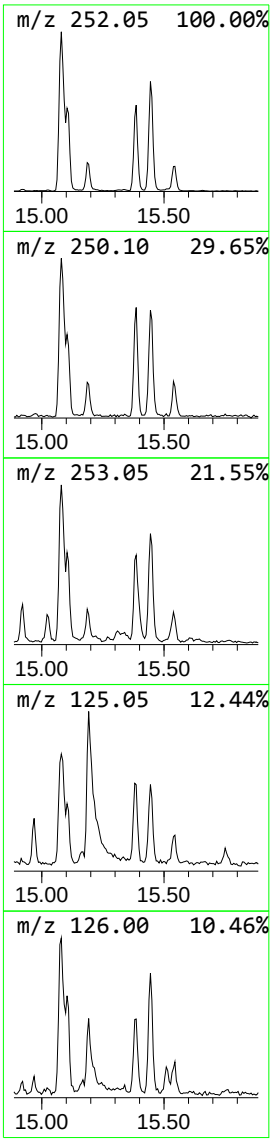
Peak Number 9 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	2.87 ng	185522	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Perylene	252	C20H12	000198-55-0	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





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ClientSampleId :
OSTL-B1

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

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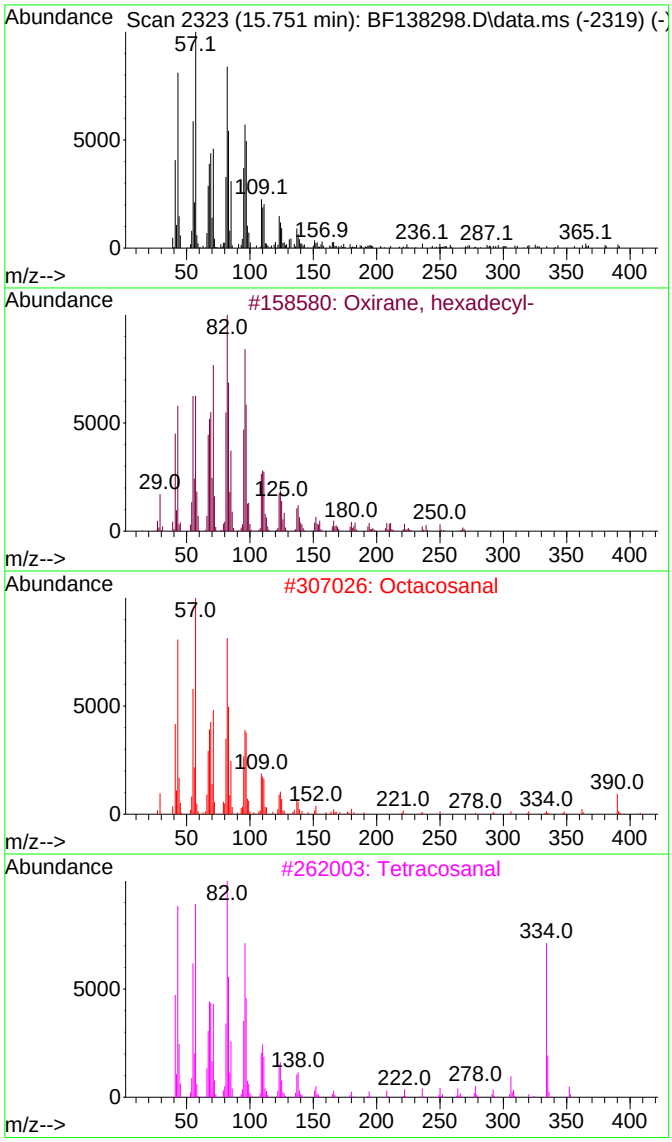
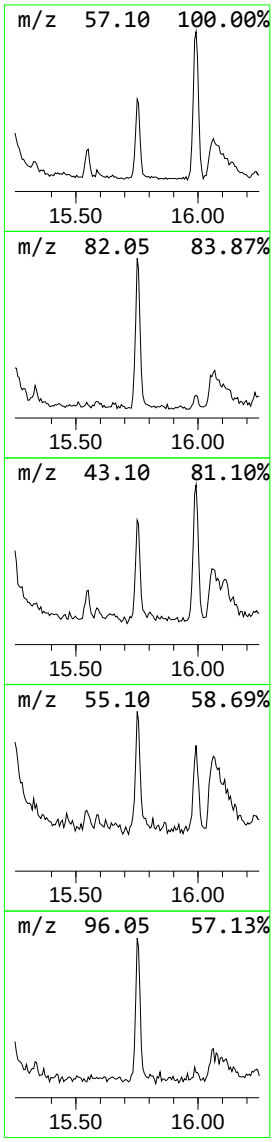
Peak Number 10 Octacosanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	4.02 ng	259943	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Octacosanal	408	C28H56O	022725-64-0	91
3	Tetracosanal	352	C24H48O	057866-08-7	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
5	1,19-Eicosadiene	278	C20H38	014811-95-1	89





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Sample : P2977-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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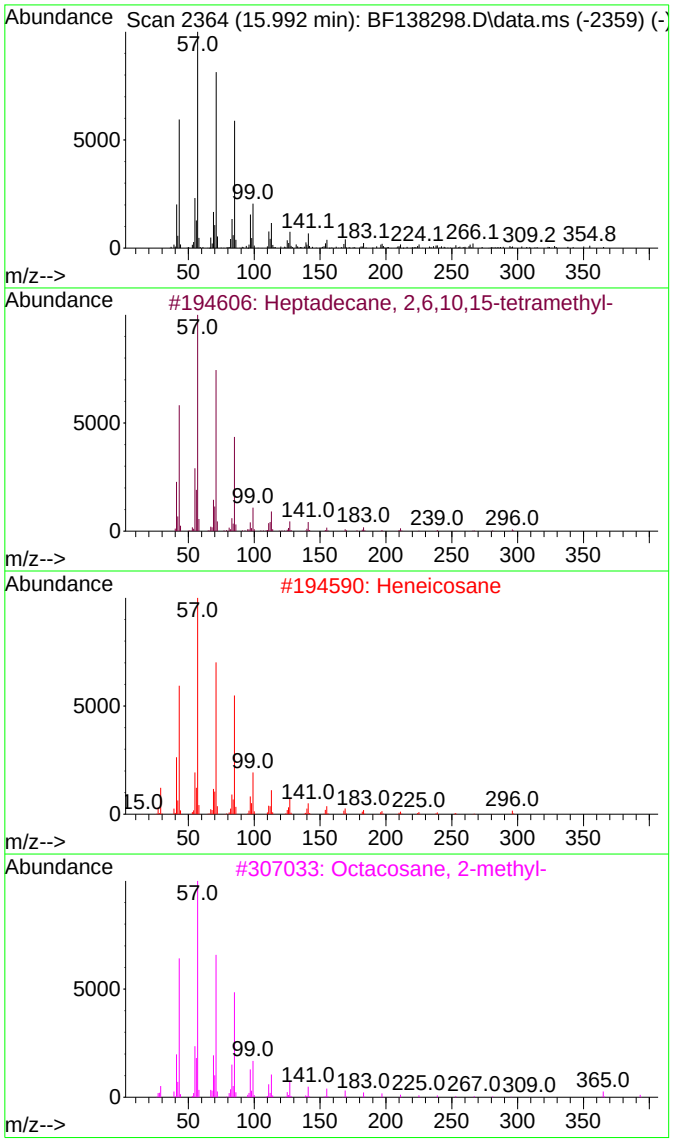
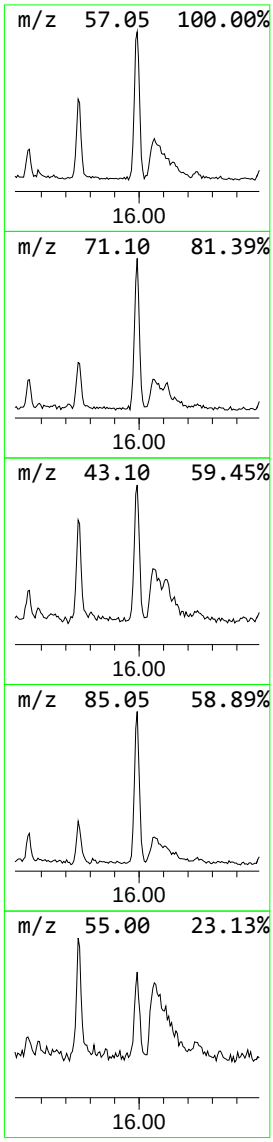
Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	4.10 ng	265325	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : P2977-07
Misc :
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Instrument :
BNA_F
ClientSampleId :
OSTL-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
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TIC Library : C:\Database\NIST20.L
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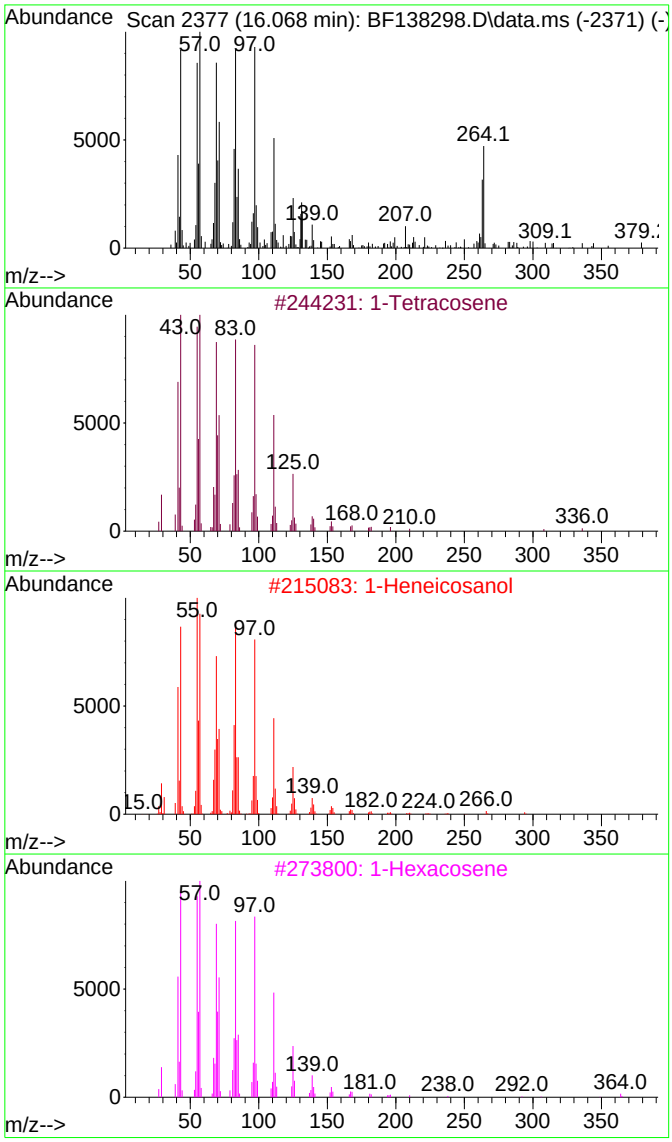
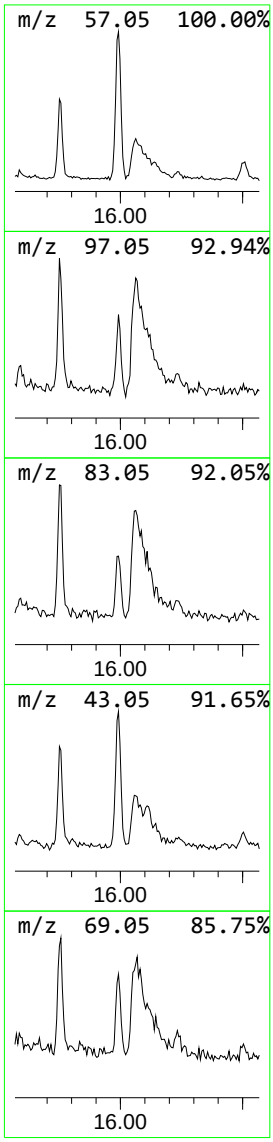
Peak Number 12 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.068	4.61 ng	298532	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Heptacos-1-ene	378	C27H54	015306-27-1	90
5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	90





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
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TIC Library : C:\Database\NIST20.L
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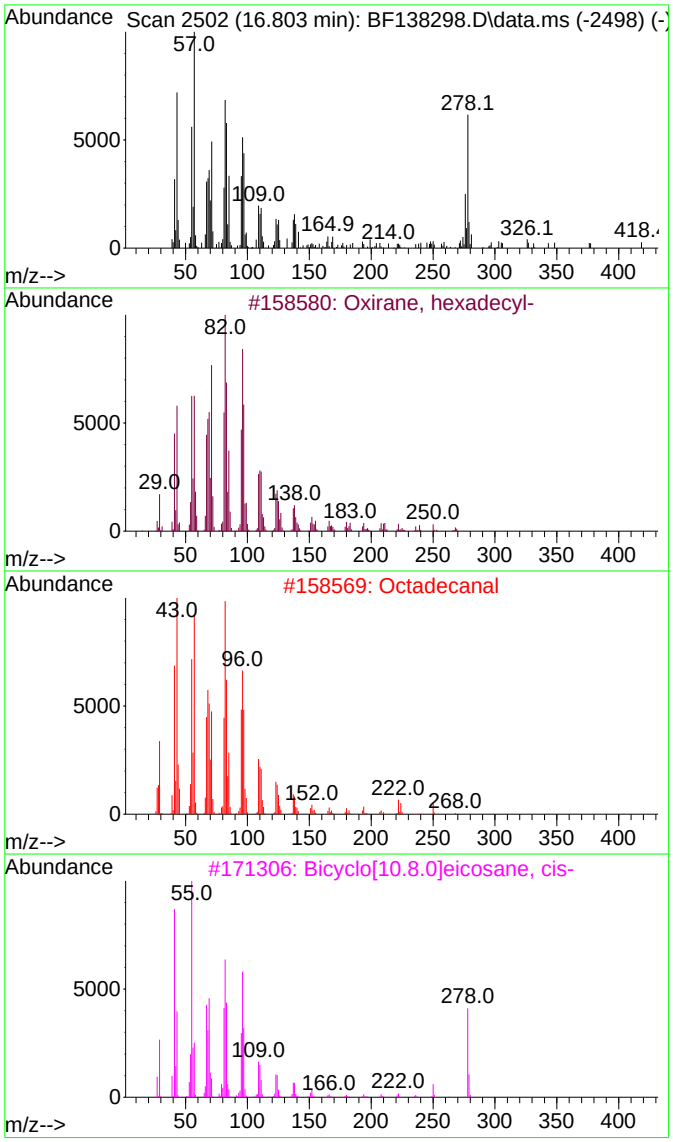
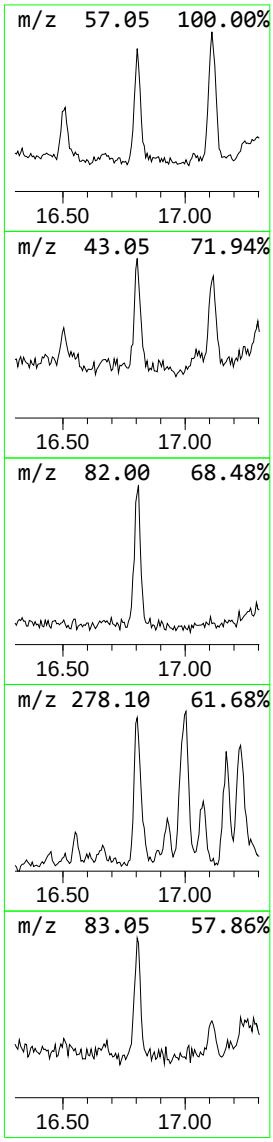
Peak Number 13 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.803	3.21 ng	207969	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2	Octadecanal	268	C18H36O	000638-66-4	86
3	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	83
4	Hexacosanal	380	C26H52O	026627-85-0	58
5	9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	52





Tentatively Identified Compound (LSC) summary

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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...	2.181	37.6	ng	3193770	1	6.886	1698820	20.0
2-Pentanone, 4-...	5.104	3.6	ng	306637	1	6.886	1698820	20.0
n-Hexadecanoic ...	11.927	7.0	ng	604964	4	11.404	1732230	20.0
Tricosyl pentaf...	13.886	4.6	ng	460871	5	14.039	2016940	20.0
Heptadecane	14.509	3.0	ng	298321	5	14.039	2016940	20.0
Oxirane, hexade...	14.968	10.5	ng	680509	6	15.509	1294340	20.0
Nonadecane	15.162	3.7	ng	241546	6	15.509	1294340	20.0
Cyclotetracosane	15.192	24.1	ng	1560650	6	15.509	1294340	20.0
Benzo[e]pyrene	15.386	2.9	ng	185522	6	15.509	1294340	20.0
Octacosanal	15.751	4.0	ng	259943	6	15.509	1294340	20.0
Heptadecane, 2,...	15.992	4.1	ng	265325	6	15.509	1294340	20.0
1-Tetracosene	16.068	4.6	ng	298532	6	15.509	1294340	20.0
Octadecanal	16.803	3.2	ng	207969	6	15.509	1294340	20.0