LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119614.D
Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	17	21	30	rVB	103567	132961	1.71%	0.194%
2	5.040	497	502	512	rVB	752541	949872	12.21%	1.383%
3	5.446	566	571	574	rBV	6507257	6350916	81.66%	9.250%
4	6.457	737	743	746	rBV	6611450	6861068	88.22%	9.993%
5	6.834	803	807	810	rBV	2158666	1798204	23.12%	2.619%
6	6.987	825	833	837	rBV	5881358	5472671	70.37%	7.971%
7	7.392	897	902	905	rBV	4725681	4578183	58.87%	6.668%
8	8.116	1020	1025	1028	rBV	2903584	2369302	30.46%	3.451%
9	9.198	1203	1209	1212	rBV	8389354	7777321	100.00%	11.327%
10	9.310	1226	1228	1232	rVB	216145	179670	2.31%	0.262%
11	9.586	1272	1275	1280	rBV	615309	487152	6.26%	0.710%
12	9.875	1318	1324	1327	rBV	3273088	2629165	33.81%	3.829%
13	9.904	1327	1329	1333	rVB	204399	167910	2.16%	0.245%
14	10.075	1355	1358	1362	rBV	86723	85441	1.10%	0.124%
15	10.422	1414	1417	1423	rBV	105782	103425	1.33%	0.151%
16	10.663	1453	1458	1461	rBV	5147475	4623079	59.44%	6.733%
17	10.786	1476	1479	1483	rBV2	68482	86560	1.11%	0.126%
18	11.104	1530	1533	1538	rVB2	169751	149048	1.92%	0.217%
19	11.363	1573	1577	1579	rBV	2891747	2531132	32.55%	3.687%
20	11.386	1579	1581	1584	rVV	664542	529411	6.81%	0.771%
21	11.433	1584	1589	1592	rVB2	108807	129855	1.67%	0.189%
22	11.757	1642	1644	1650	rVB	120591	114911	1.48%	0.167%
23	11.892	1664	1667	1673	rBV	1255396	1150259	14.79%	1.675%
24	11.975	1679	1681	1683	rVB	166463	116883	1.50%	0.170%
25	12.445	1758	1761	1763	rBV2	260601	268681	3.45%	0.391%
26	12.469	1763	1765	1767	rVB	270366	223609	2.88%	0.326%
27	12.574	1776	1783	1786	rBV	1058122	1012074	13.01%	1.474%
28	12.622	1789	1791	1797	rVB2	150820	144113	1.85%	0.210%
29	12.674	1797	1800	1807	rBV	445979	533606	6.86%	0.777%
30	12.804	1814	1822	1824	rBV	695249	830093	10.67%	1.209%
31	12.851	1828	1830	1836	rVB3	88139	94133	1.21%	0.137%
32	12.951	1842	1847	1850	rBV	6931002	6238622	80.22%	9.086%
33	13.133	1872	1878	1881	rVB2	103700	134212	1.73%	0.195%
34	13.198	1885	1889	1892	rBV2	116713	142047	1.83%	0.207%

LSC Area Percent Report

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Sample : L2040-01
Misc :
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Instrument : BNA_F
ClientSampleId : RO-350

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.433	1925	1929	1931	rBV	271305	245809	3.16%	0.358%
36	13.868	1998	2003	2017	rBV6	261698	748947	9.63%	1.091%
37	13.998	2020	2025	2028	rVV	1801715	1975963	25.41%	2.878%
38	14.021	2028	2029	2032	rVB	183988	141192	1.82%	0.206%
39	14.174	2051	2055	2060	rBV	346390	303739	3.91%	0.442%
40	14.480	2103	2107	2110	rBV	532607	496216	6.38%	0.723%
41	14.786	2155	2159	2166	rVB	651611	639821	8.23%	0.932%
42	14.863	2169	2172	2178	rVB	161531	180263	2.32%	0.263%
43	15.033	2197	2201	2205	rBV	219525	347711	4.47%	0.506%
44	15.121	2212	2216	2223	rBV	595813	751449	9.66%	1.094%
45	15.339	2249	2253	2256	rBV	110167	144464	1.86%	0.210%
46	15.398	2260	2263	2267	rVV	129637	144180	1.85%	0.210%
47	15.463	2269	2274	2278	rVV	1330889	1649750	21.21%	2.403%
48	15.510	2278	2282	2287	rVB	518638	713140	9.17%	1.039%
49	15.945	2351	2356	2362	rBV	375528	548429	7.05%	0.799%
50	16.451	2437	2442	2453	rVB	196560	382268	4.92%	0.557%
51	16.909	2517	2520	2531	rVB3	59310	110673	1.42%	0.161%
52	17.051	2540	2544	2549	rVB3	69163	139795	1.80%	0.204%

Sum of corrected areas: 68659398

LSC Report - Integrated Chromatogram

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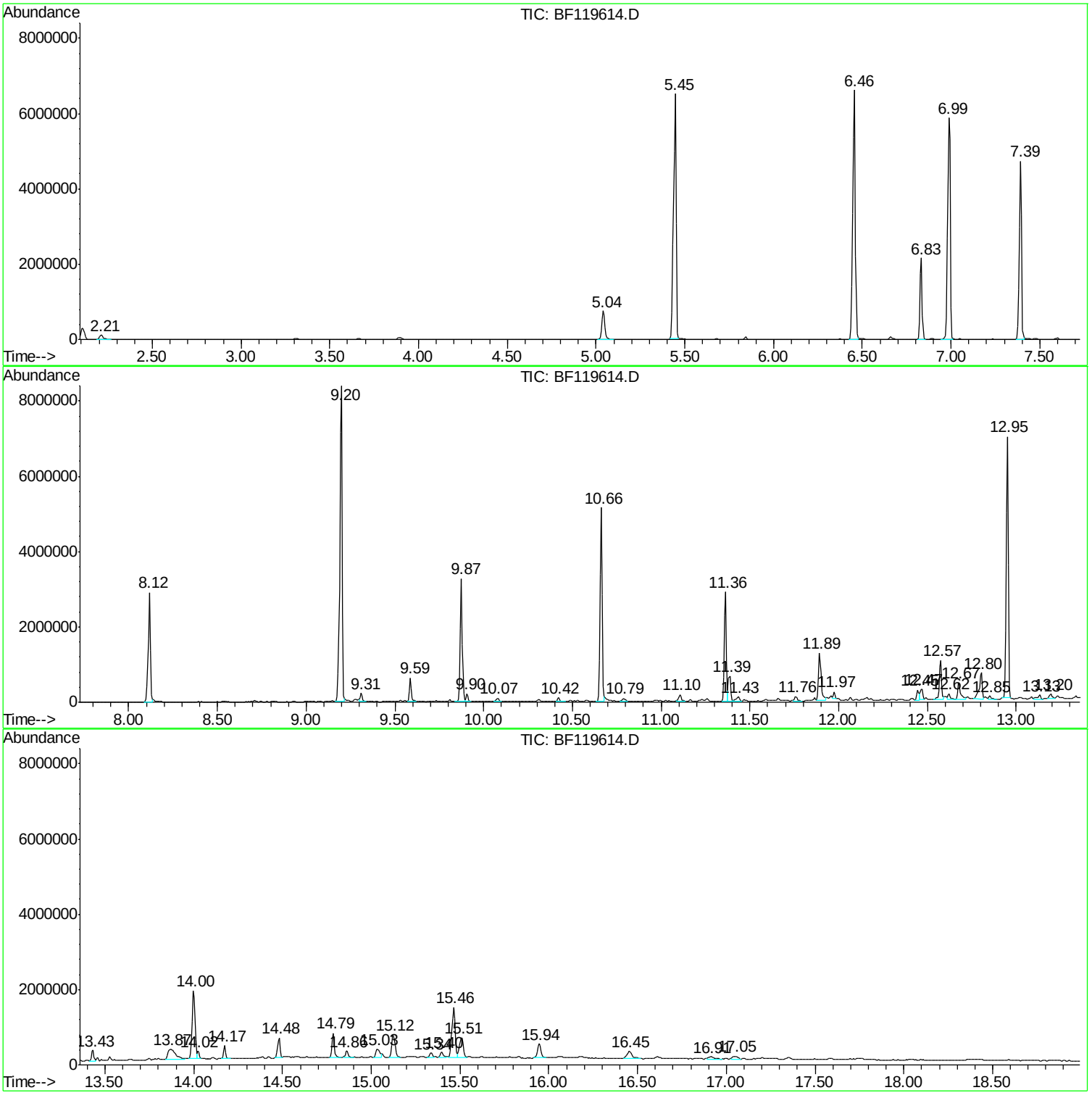
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119614.D
Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

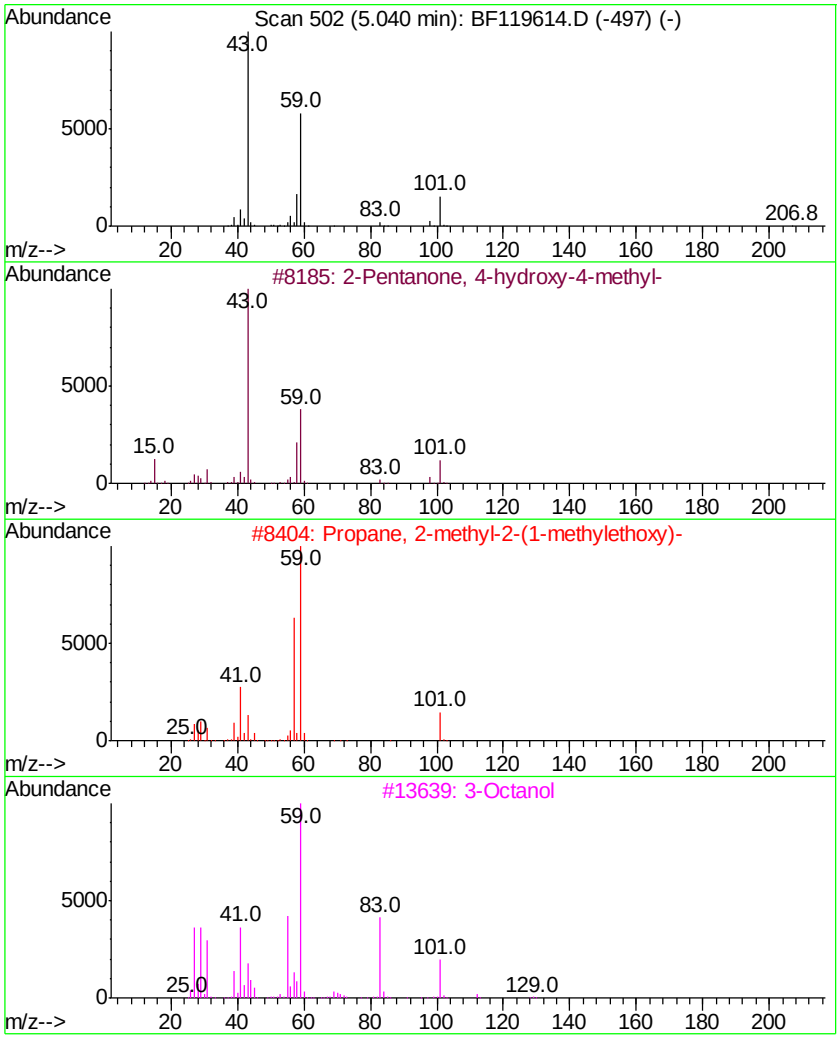
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

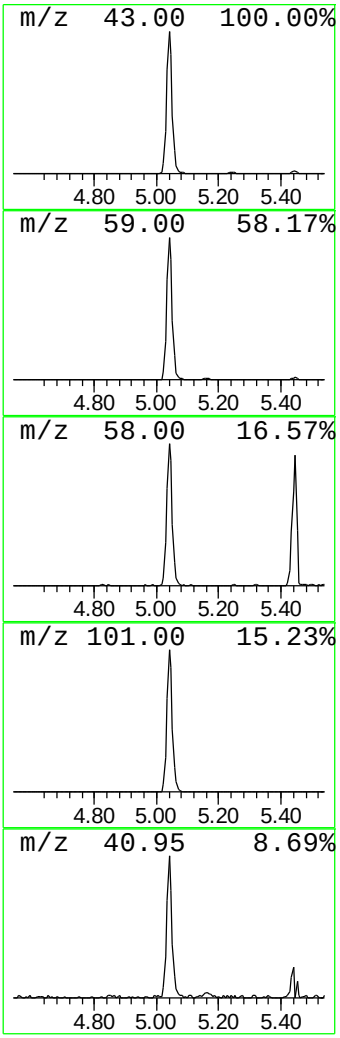
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	10.56 ng	949872	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Library Search Compound Report

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Data File : BF119614.D
Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

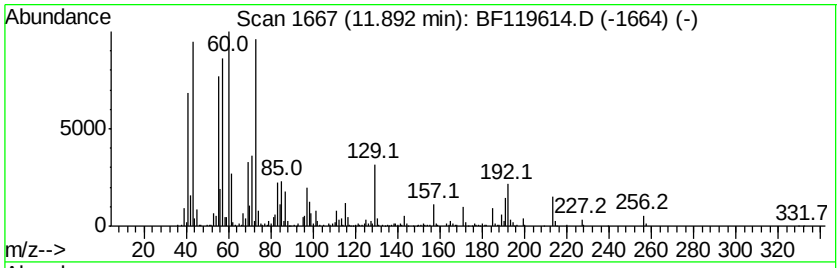
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

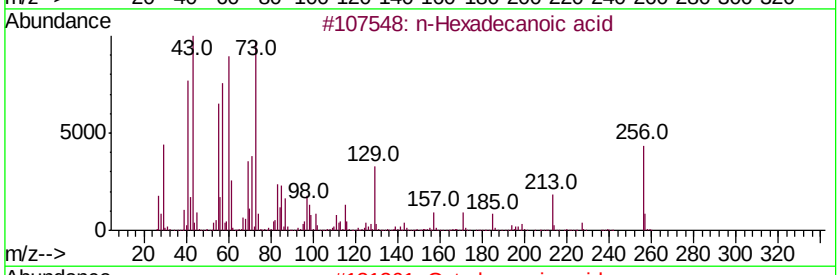
****

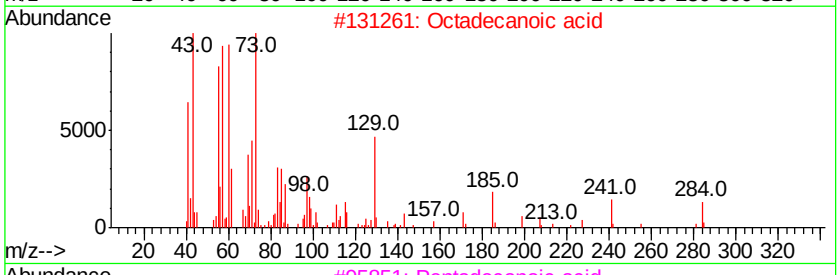
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

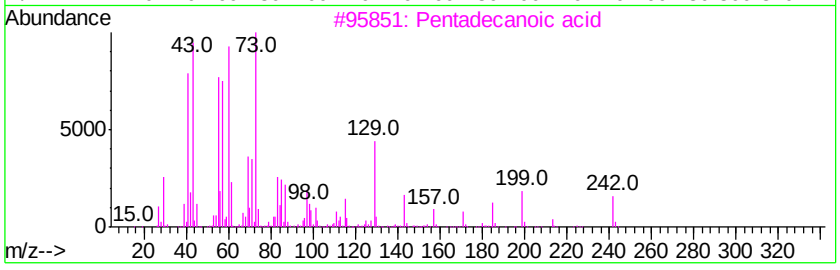
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	9.09 ng	1150260	Phenanthrene-d10	11.36

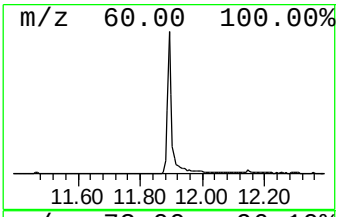
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64

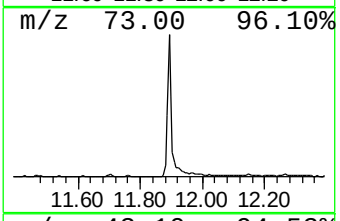


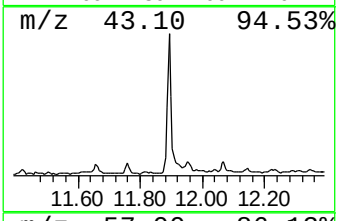


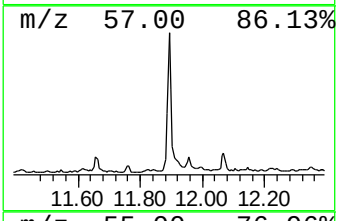


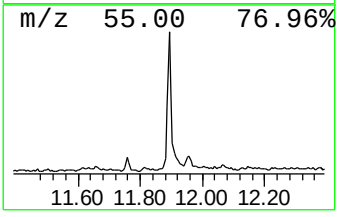












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Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

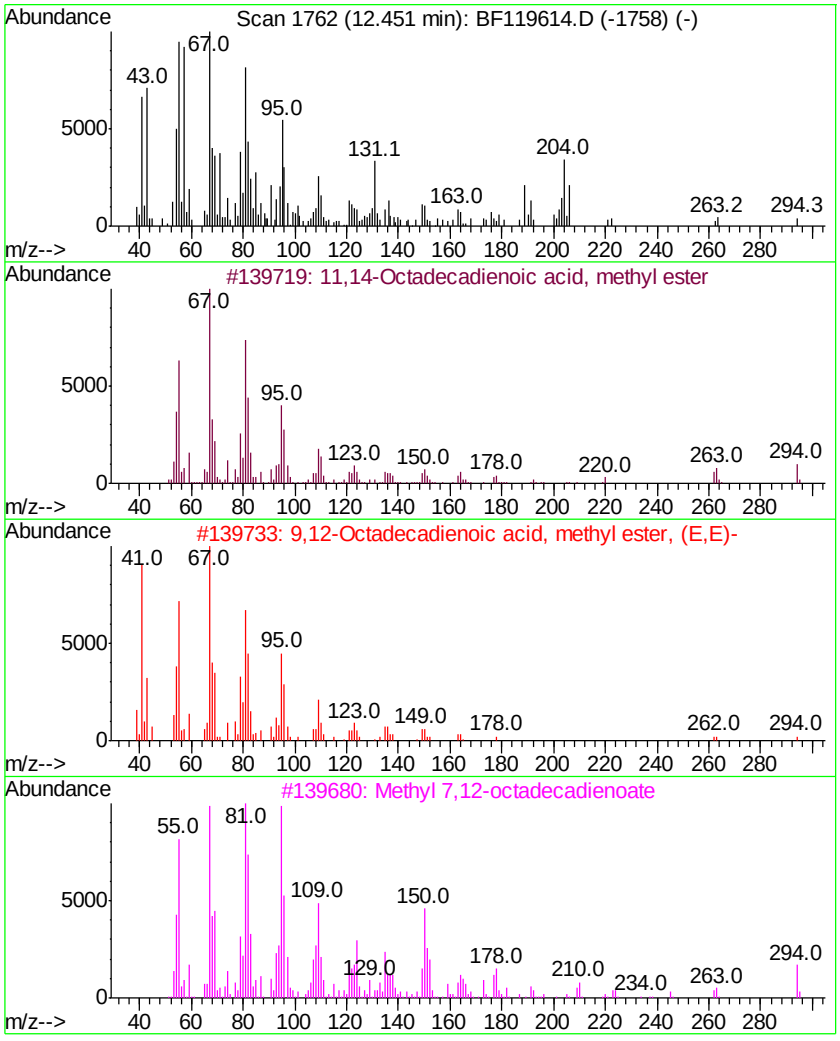
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

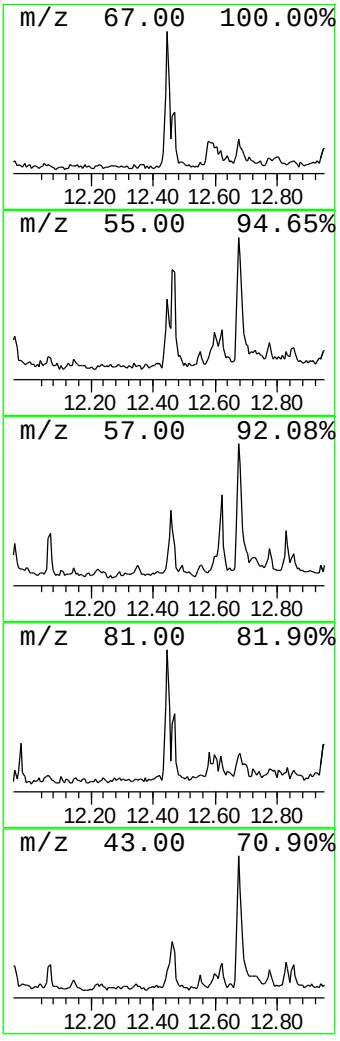
****

Peak Number 4 11,14-Octadecadienoic acid,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	2.12 ng	268681	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	96
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	96
3	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	94
4	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	91





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

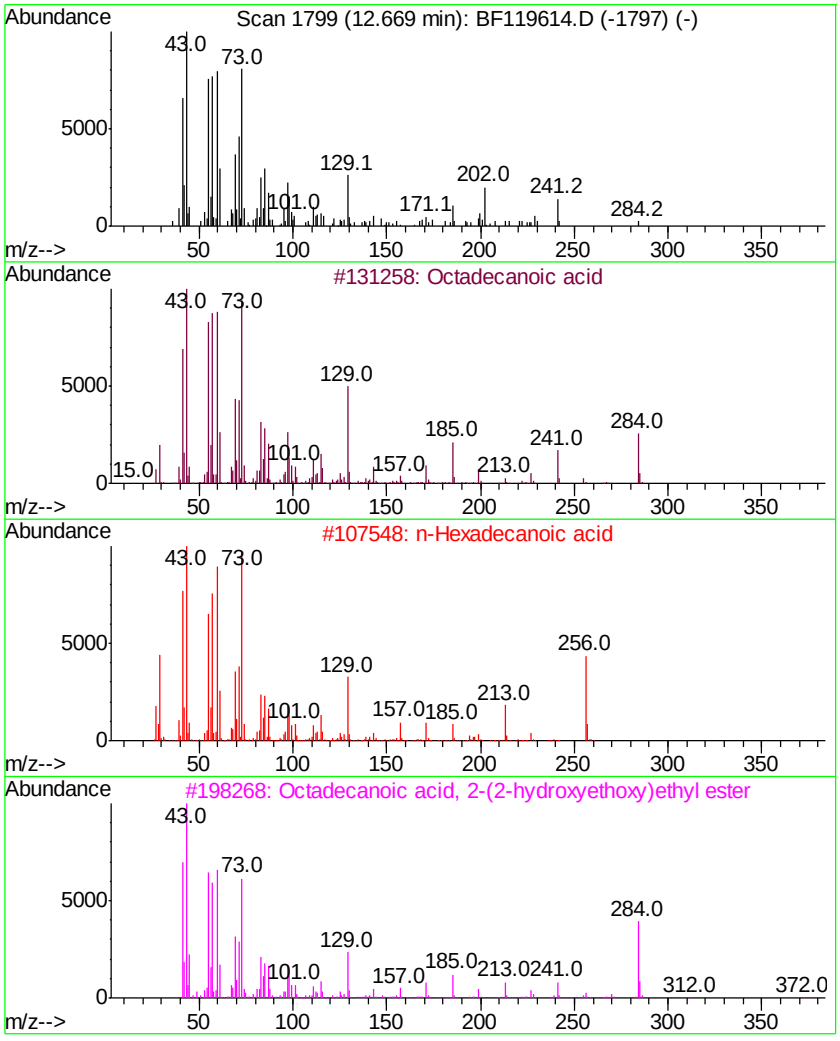
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

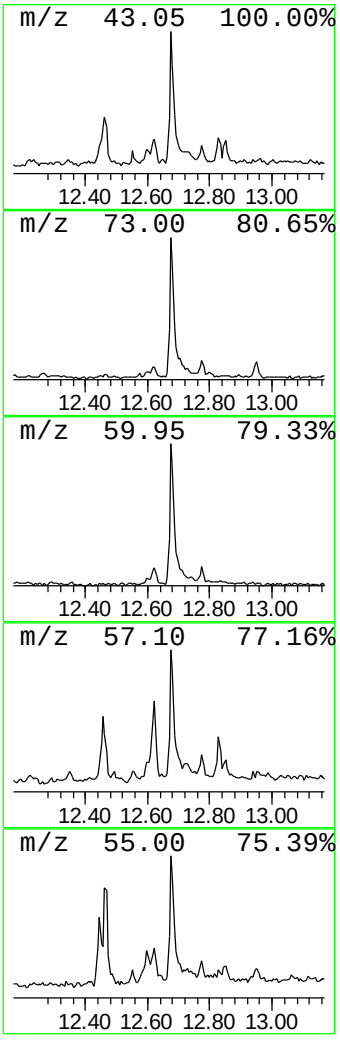
****

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	4.22 ng	533606	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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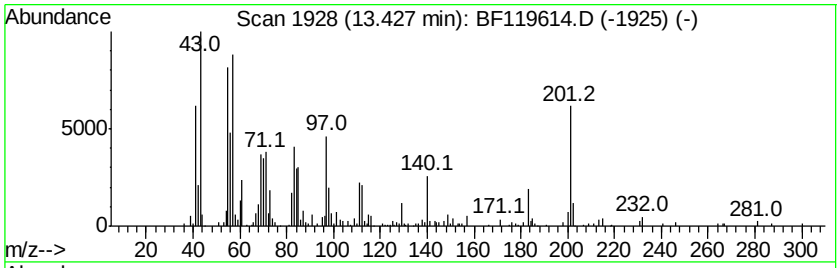
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

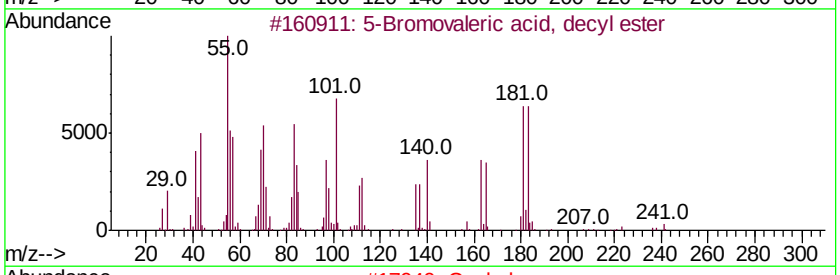
****

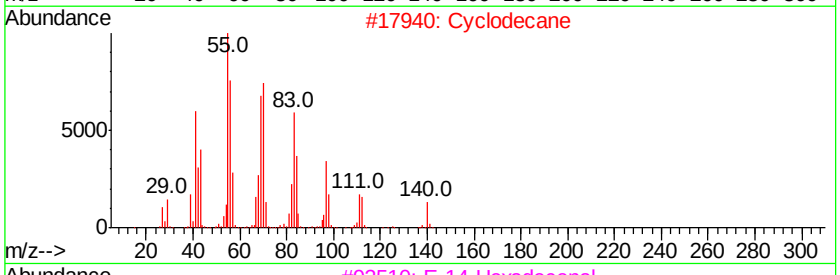
Peak Number 6 unknown13.43 Concentration Rank 12

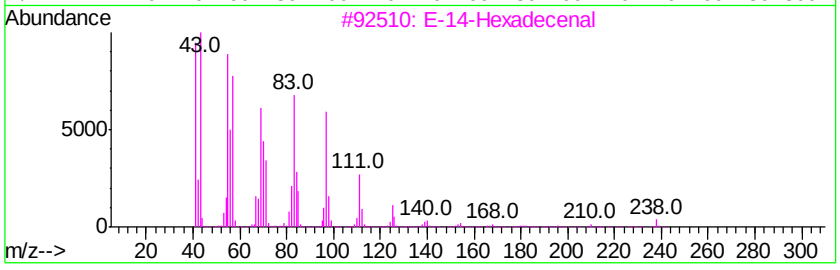
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	2.49 ng	245809	Chrysene-d12	14.00

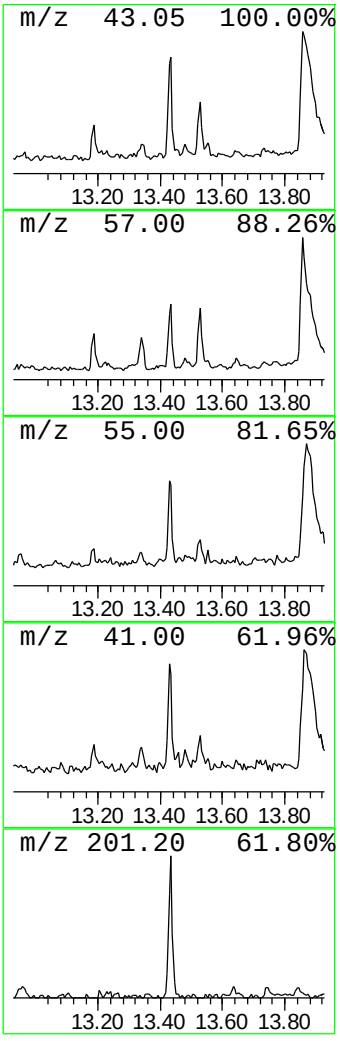
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromovaleric acid, decyl ester	320	C15H29BrO2	175083-30-4	46
2	Cyclodecane	140	C10H20	000293-96-9	41
3	E-14-Hexadecenal	238	C16H30O	330207-53-9	38
4	1-Hexene-3,5-dione	112	C6H8O2	052204-69-0	38
5	1-Dodecanethiol	202	C12H26S	000112-55-0	38











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Sample : L2040-01
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

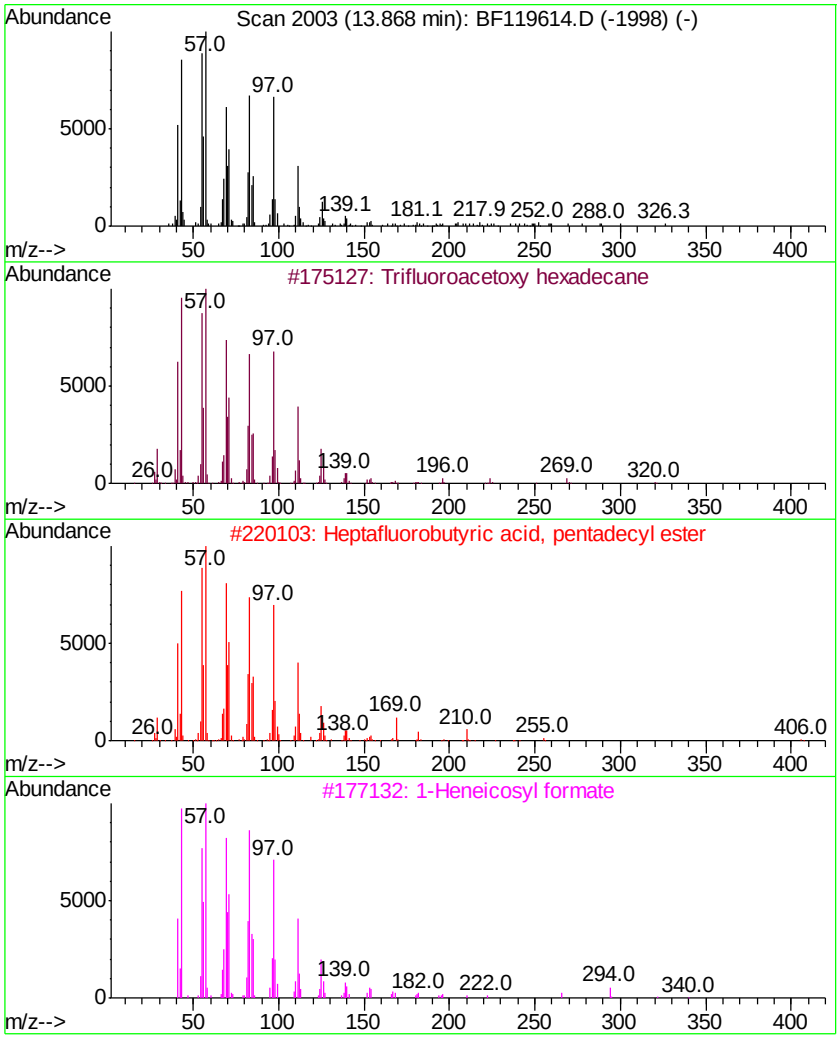
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

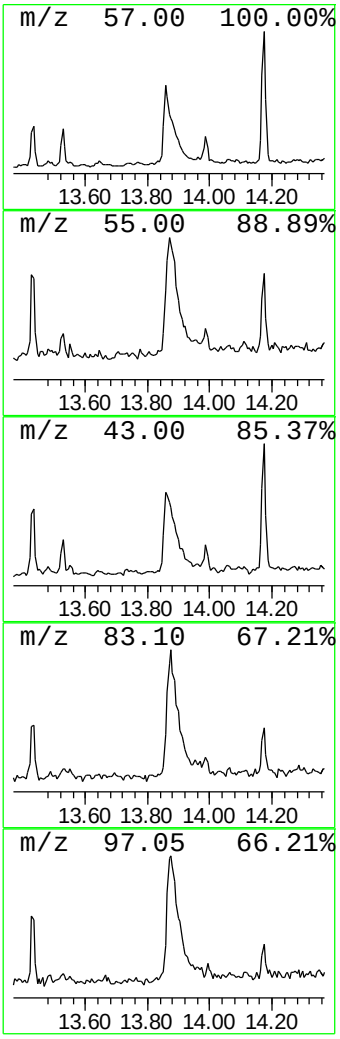
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.58 ng	748947	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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Data File : BF119614.D
Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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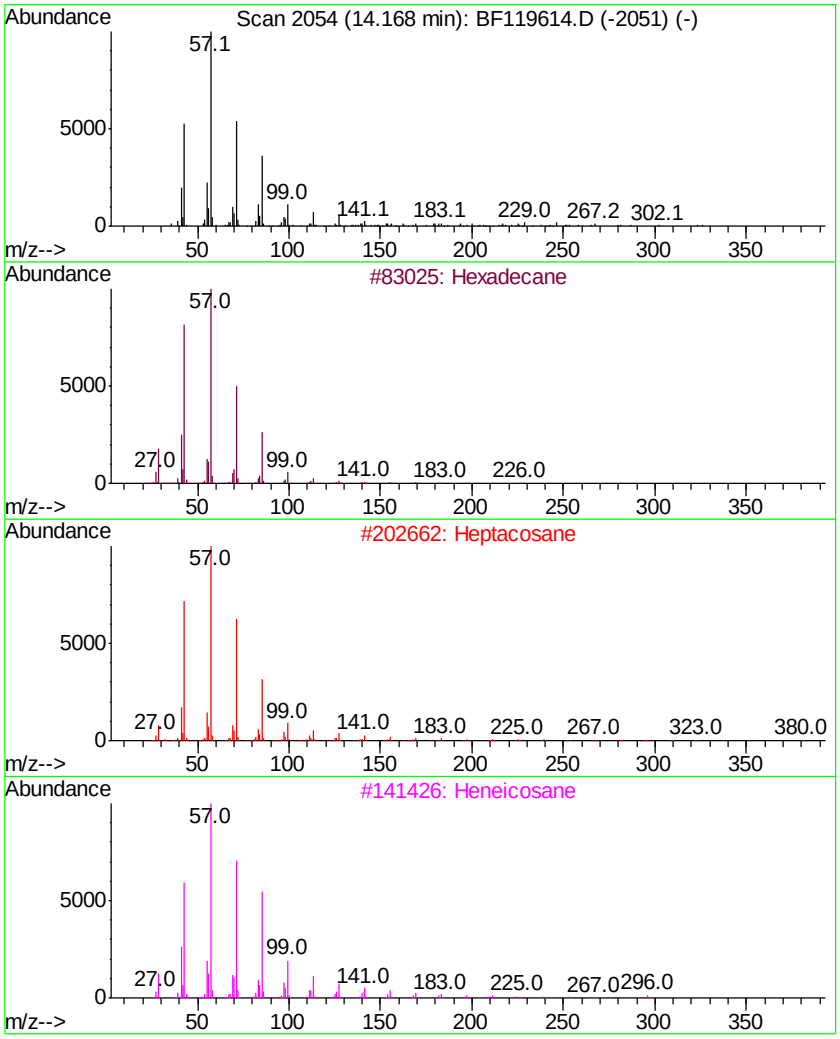
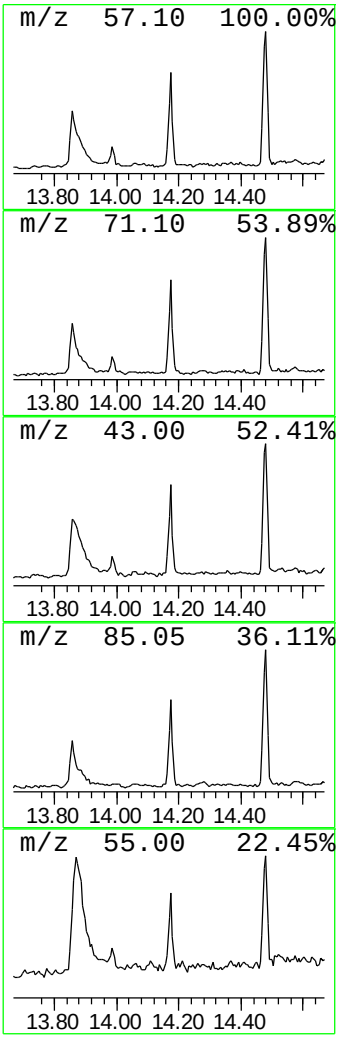
Peak Number 8 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	3.07 ng	303739	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	86





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Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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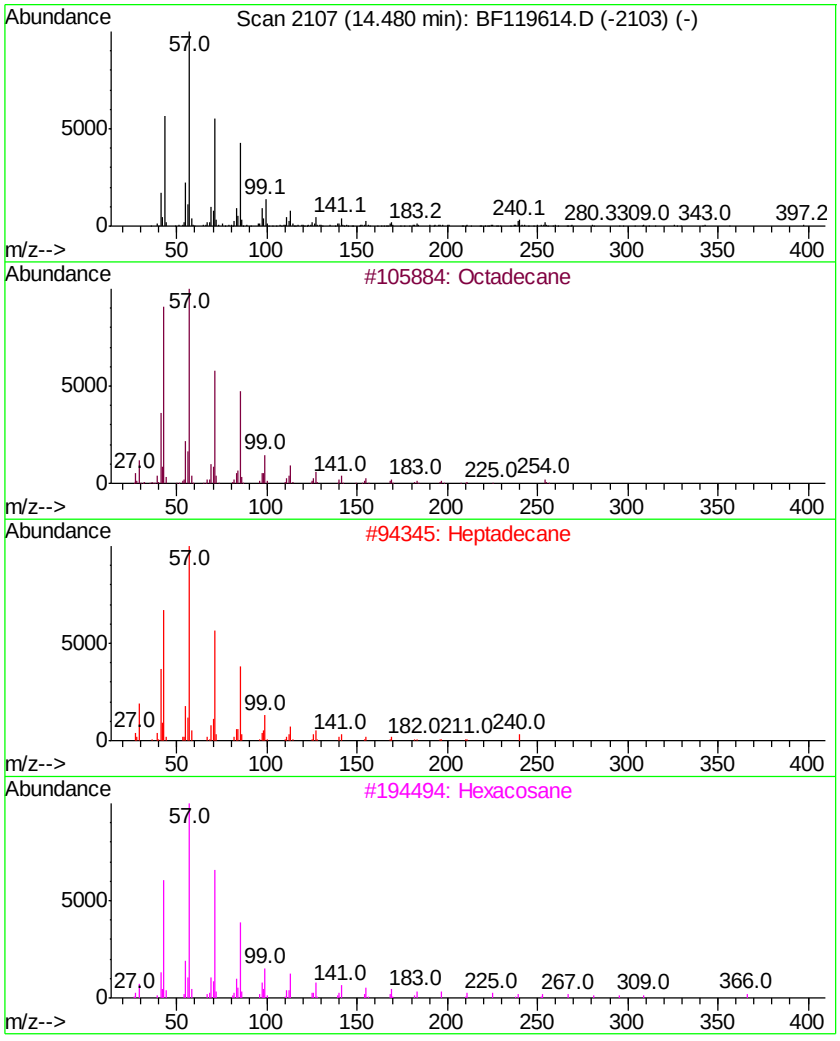
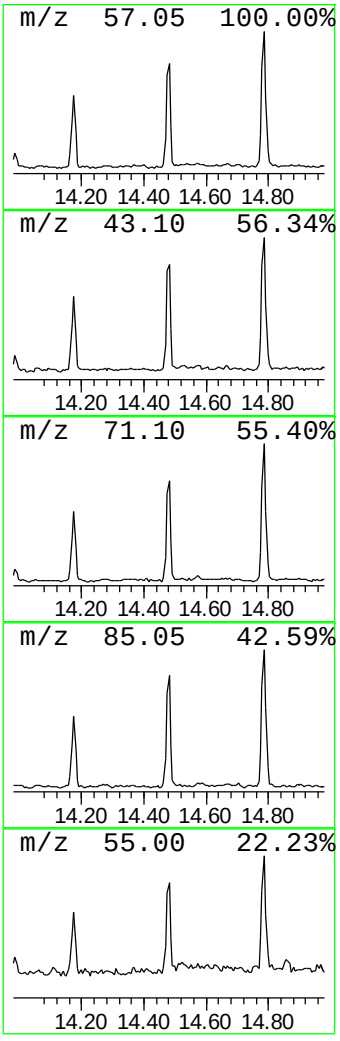
Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	5.02 ng	496216	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Heptadecane	240	C17H36	000629-78-7	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heneicosane	296	C21H44	000629-94-7	87





Library Search Compound Report

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Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

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TIC Library : C:\DATABASE\NIST11.L
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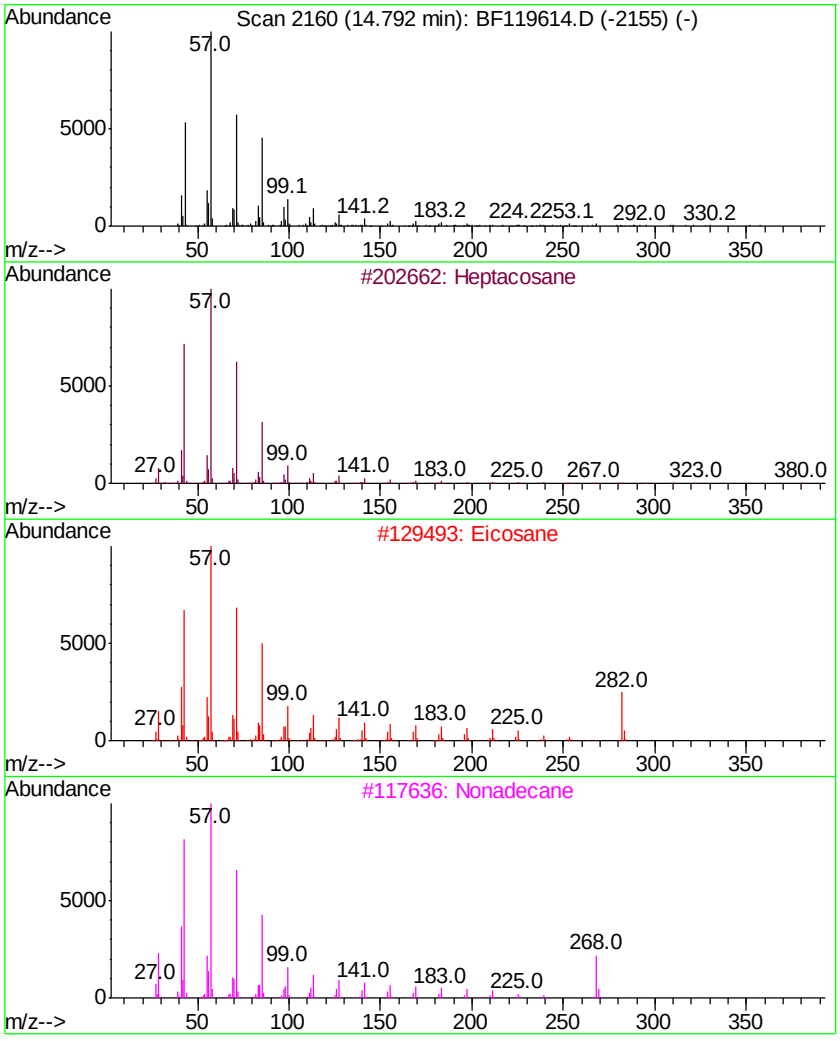
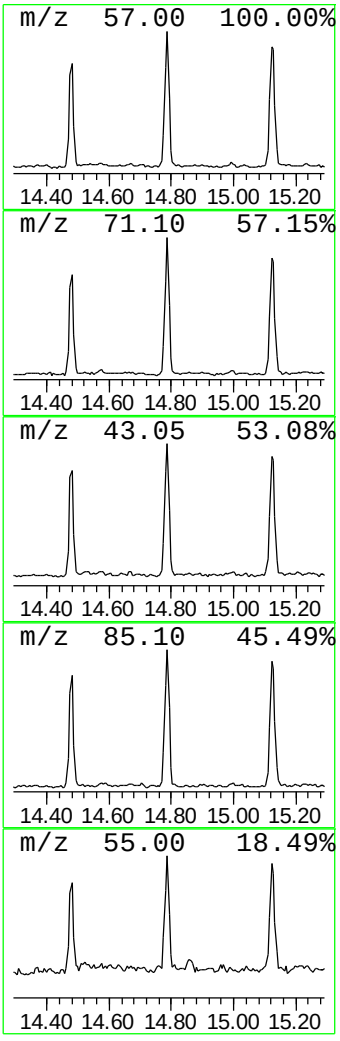
Peak Number 10 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	7.76 ng	639821	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Nonadecane	268	C19H40	000629-92-5	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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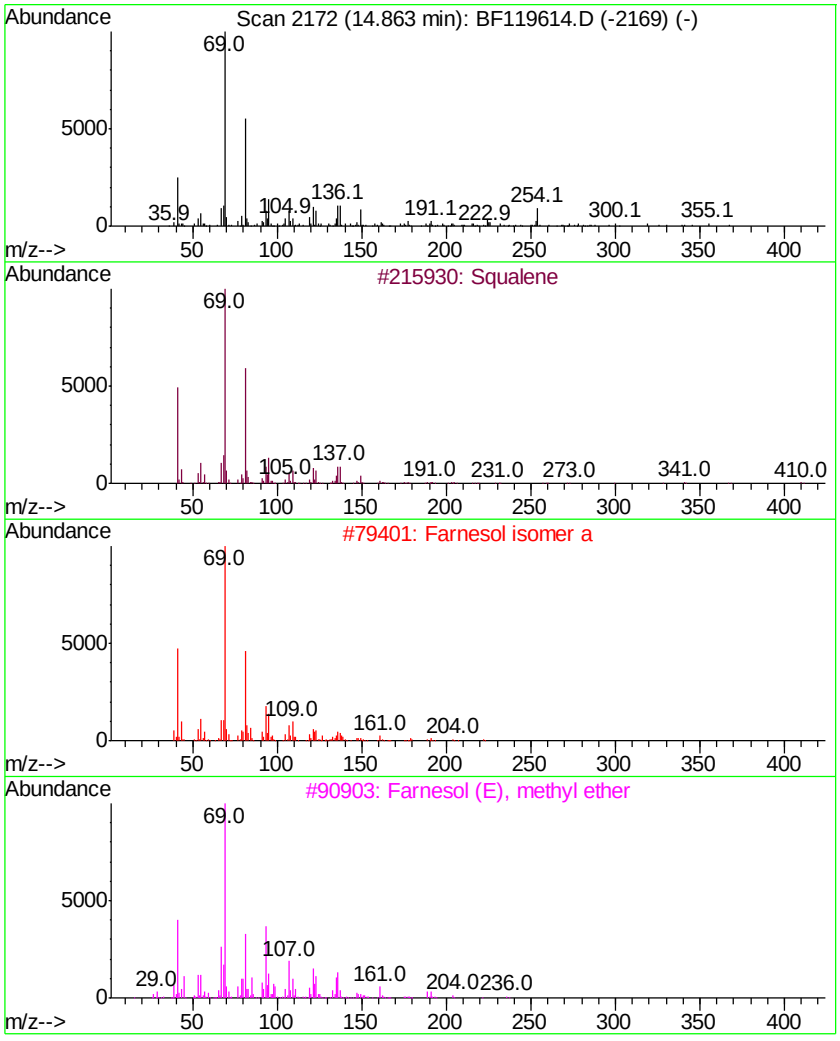
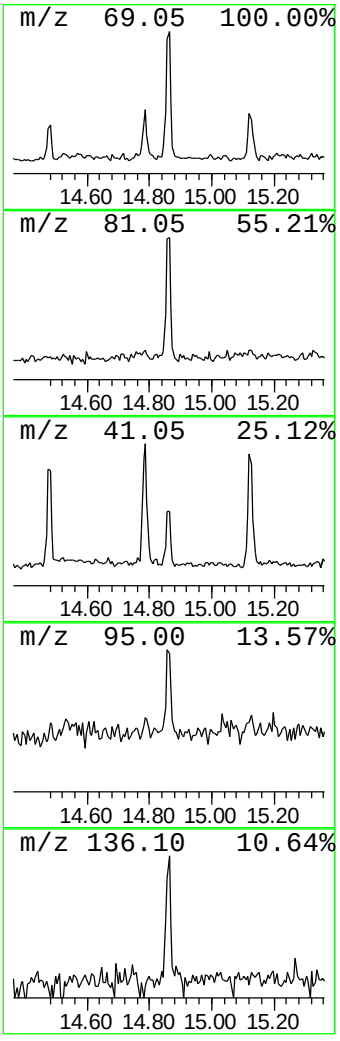
Peak Number 11 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.19 ng	180263	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	Farnesol isomer a	222	C15H26O	1000108-92-4	76
3	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	58





Library Search Compound Report

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Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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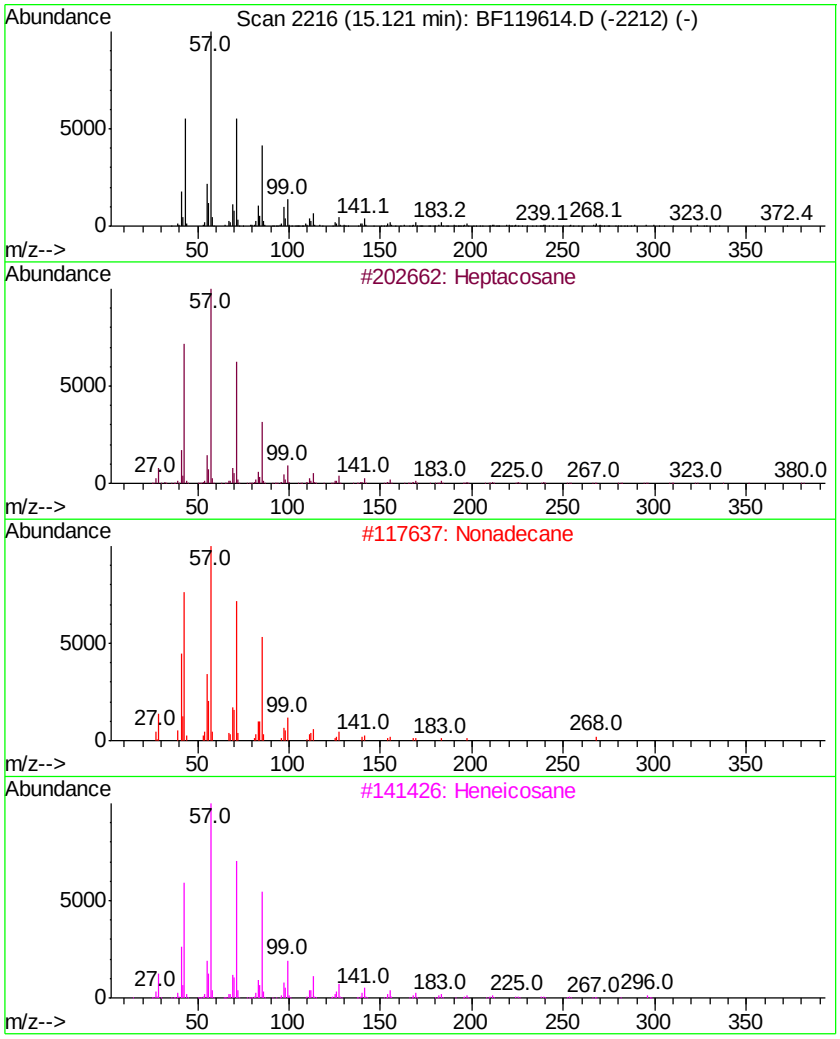
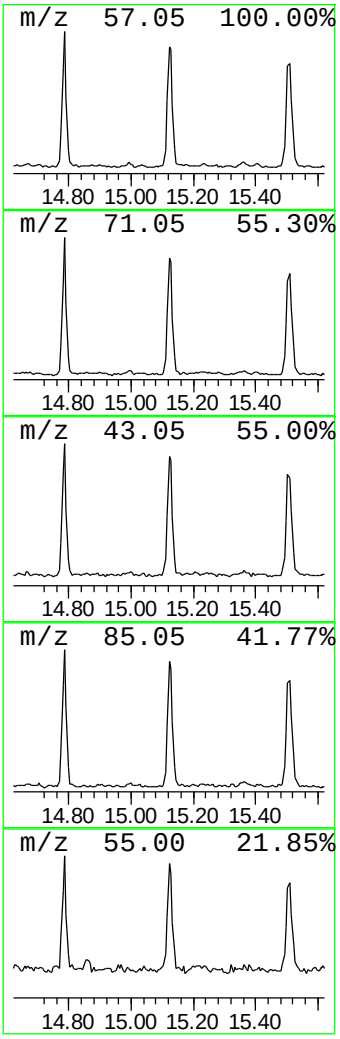
Peak Number 12 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	9.11 ng	751449	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Pentadecane	212	C15H32	000629-62-9	83





Library Search Compound Report

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Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
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TIC Integration Parameters: LSCINT.P

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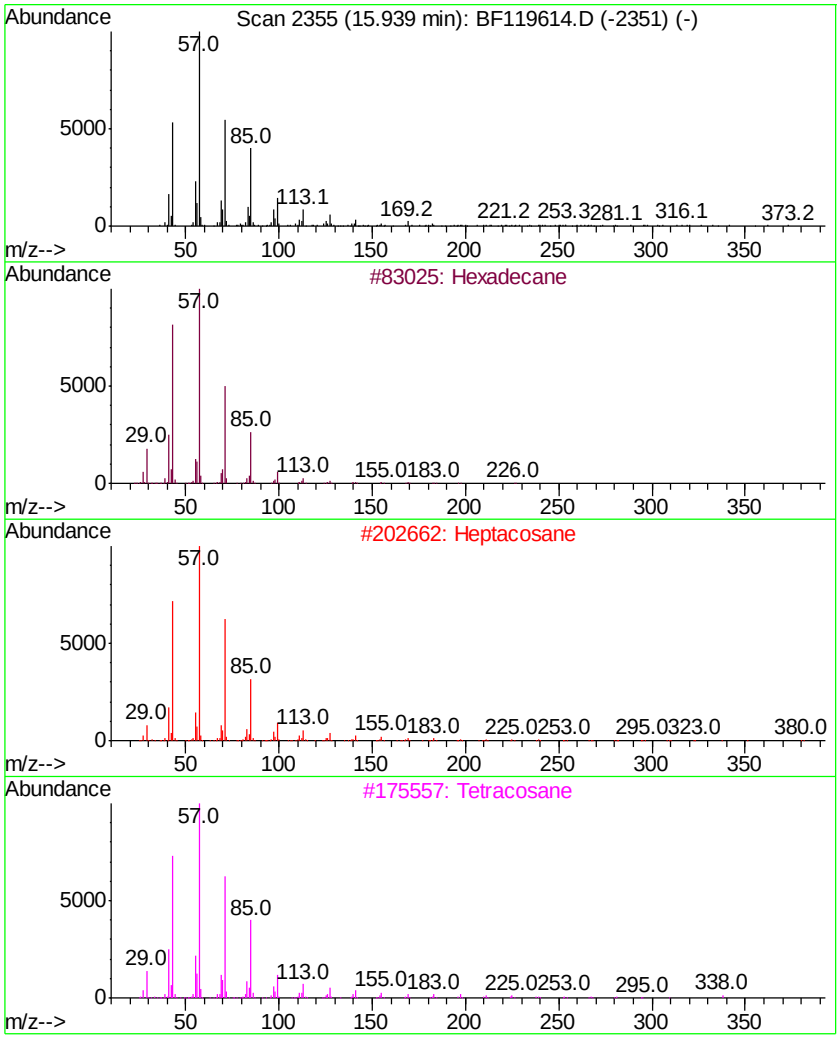
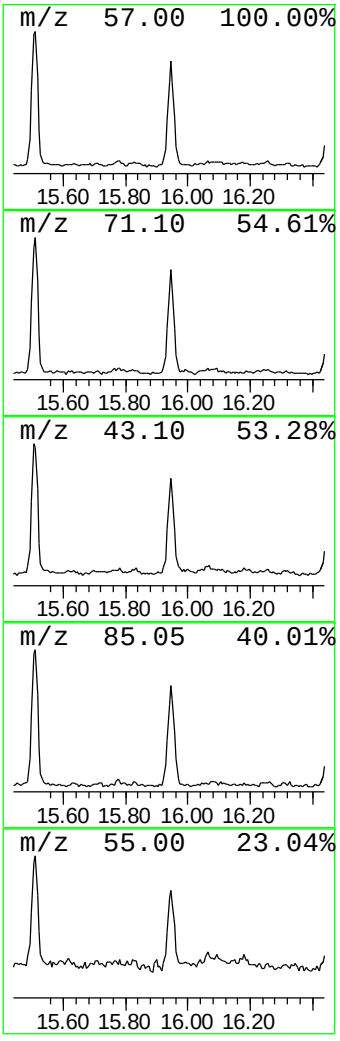
Peak Number 13 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	6.65 ng	548429	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Docosane	310	C22H46	000629-97-0	90





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Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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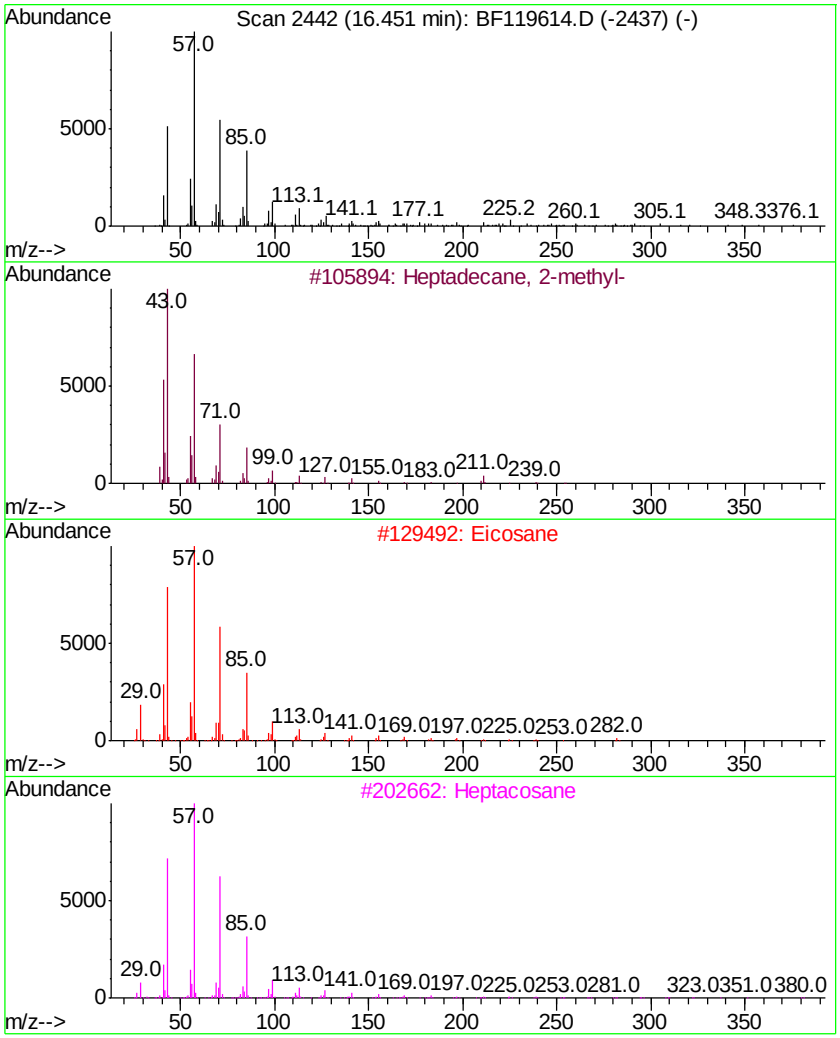
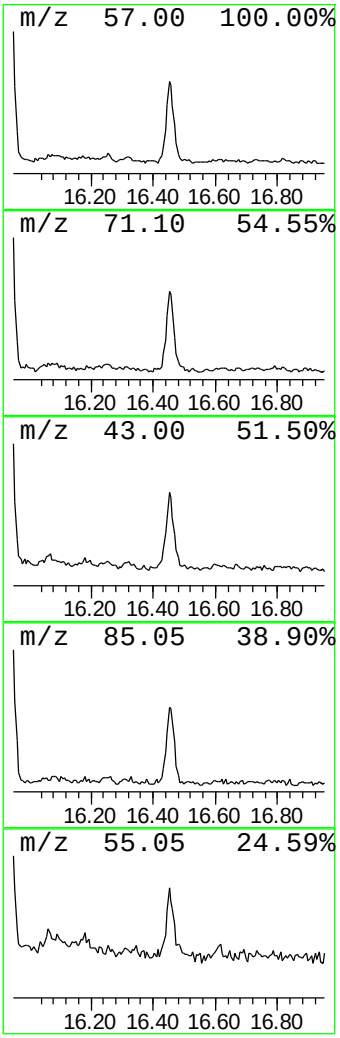
Peak Number 14 Heptadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	4.63 ng	382268	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
5	1-Iodoundecane	282	C11H23I	004282-44-4	87





Tentatively Identified Compound (LSC) summary

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Data File : BF119614.D
Acq On : 28 Mar 2020 14:03
Operator : CG/JU
Sample : L2040-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-350

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	10.6	ng	949872	1	6.83	1798200	20.0
n-Hexadecanoic acid	11.89	9.1	ng	1150260	4	11.36	2531130	20.0
11,14-Octadecadie...	12.45	2.1	ng	268681	4	11.36	2531130	20.0
Octadecanoic acid	12.67	4.2	ng	533606	4	11.36	2531130	20.0
unknown13.43	13.43	2.5	ng	245809	5	14.00	1975960	20.0
Trifluoroacetoxy ...	13.87	7.6	ng	748947	5	14.00	1975960	20.0
Hexadecane	14.17	3.1	ng	303739	5	14.00	1975960	20.0
Octadecane	14.48	5.0	ng	496216	5	14.00	1975960	20.0
Heptacosane	14.79	7.8	ng	639821	6	15.46	1649750	20.0
Squalene	14.86	2.2	ng	180263	6	15.46	1649750	20.0
Nonadecane	15.12	9.1	ng	751449	6	15.46	1649750	20.0
Tetracosane	15.94	6.7	ng	548429	6	15.46	1649750	20.0
Heptadecane, 2-me...	16.45	4.6	ng	382268	6	15.46	1649750	20.0