LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116749.D
Acq On : 1 Sep 2019 18:15
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

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-BF083019.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	5.457	568	573	576	rBV	1398909	1395392	73.40%	8.482%
2	6.469	741	745	757	rBV	1695399	1609579	84.67%	9.784%
3	6.610	765	769	773	rBV	1746030	1550885	81.58%	9.427%
4	6.845	805	809	812	rBV	553427	432714	22.76%	2.630%
5	7.004	832	836	839	rBV	1245318	1103489	58.05%	6.708%
6	7.398	899	903	906	rBV	1097557	926515	48.74%	5.632%
7	8.128	1023	1027	1030	rBV	741480	578113	30.41%	3.514%
8	9.198	1206	1209	1212	rBV	1982613	1544326	81.24%	9.387%
9	9.586	1272	1275	1281	rBV	130493	121039	6.37%	0.736%
10	9.881	1321	1325	1328	rBV	822952	728861	38.34%	4.430%
11	10.663	1454	1458	1469	rBV	1194214	1071549	56.37%	6.513%
12	11.357	1573	1576	1579	rBV	958358	824364	43.36%	5.011%
13	11.886	1663	1666	1669	rBV2	63131	64775	3.41%	0.394%
14	12.569	1779	1782	1785	rVB	84281	77211	4.06%	0.469%
15	12.792	1818	1820	1824	rVB	63315	57603	3.03%	0.350%
16	12.939	1841	1845	1848	rBV	2253076	1901008	100.00%	11.555%
17	13.833	1994	1997	2006	rVB	313338	351128	18.47%	2.134%
18	13.986	2019	2023	2027	rBV	799133	769177	40.46%	4.675%
19	14.157	2050	2052	2057	rVB2	52401	48950	2.57%	0.298%
20	14.463	2101	2104	2107	rBV2	97336	105254	5.54%	0.640%
21	14.763	2153	2155	2162	rVV2	80902	86744	4.56%	0.527%
22	14.839	2165	2168	2174	rVB	80473	89852	4.73%	0.546%
23	15.098	2209	2212	2215	rBV	93318	100374	5.28%	0.610%
24	15.439	2266	2270	2274	rBV	548582	695662	36.59%	4.229%
25	15.474	2274	2276	2285	rVB2	95092	127306	6.70%	0.774%
26	15.904	2346	2349	2353	rBV2	60794	89537	4.71%	0.544%

Sum of corrected areas: 16451407

LSC Report - Integrated Chromatogram

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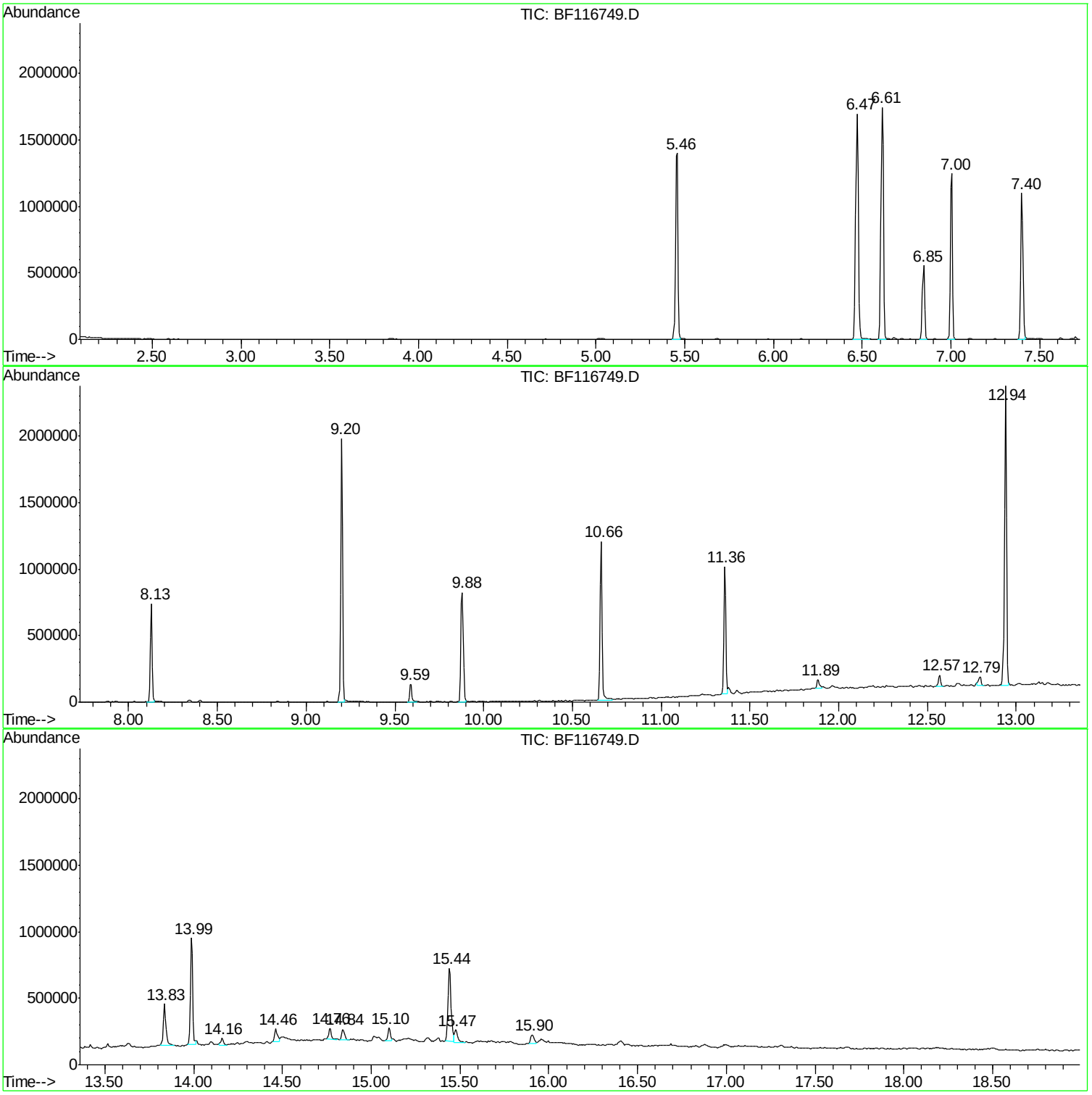
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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\BF090119\
Data File : BF116749.D
Acq On : 1 Sep 2019 18:15
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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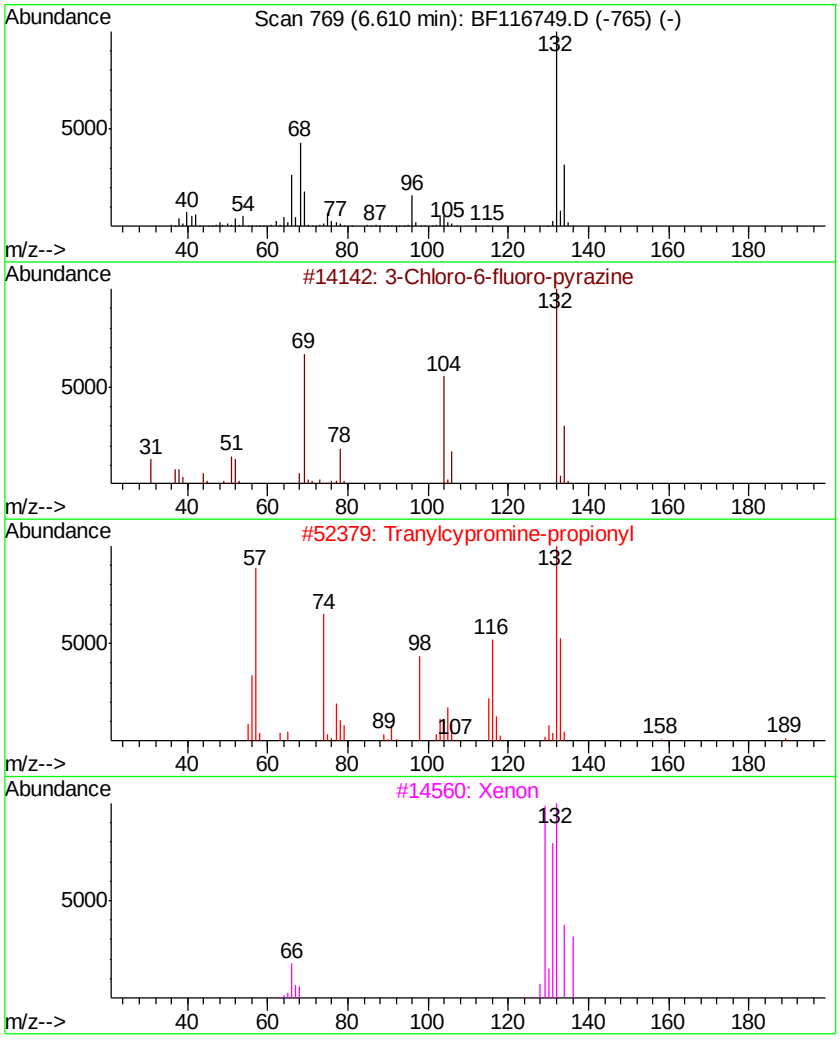
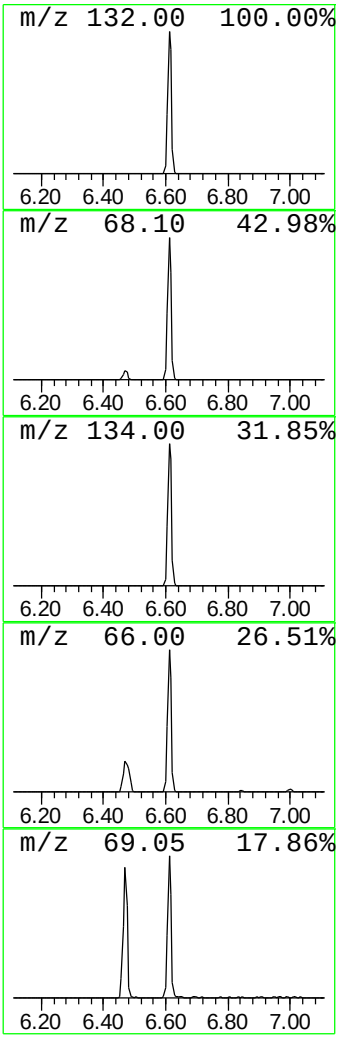
Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	71.68 ng	1550890	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Xenon	132	Xe	007440-63-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF116749.D
Acq On : 1 Sep 2019 18:15
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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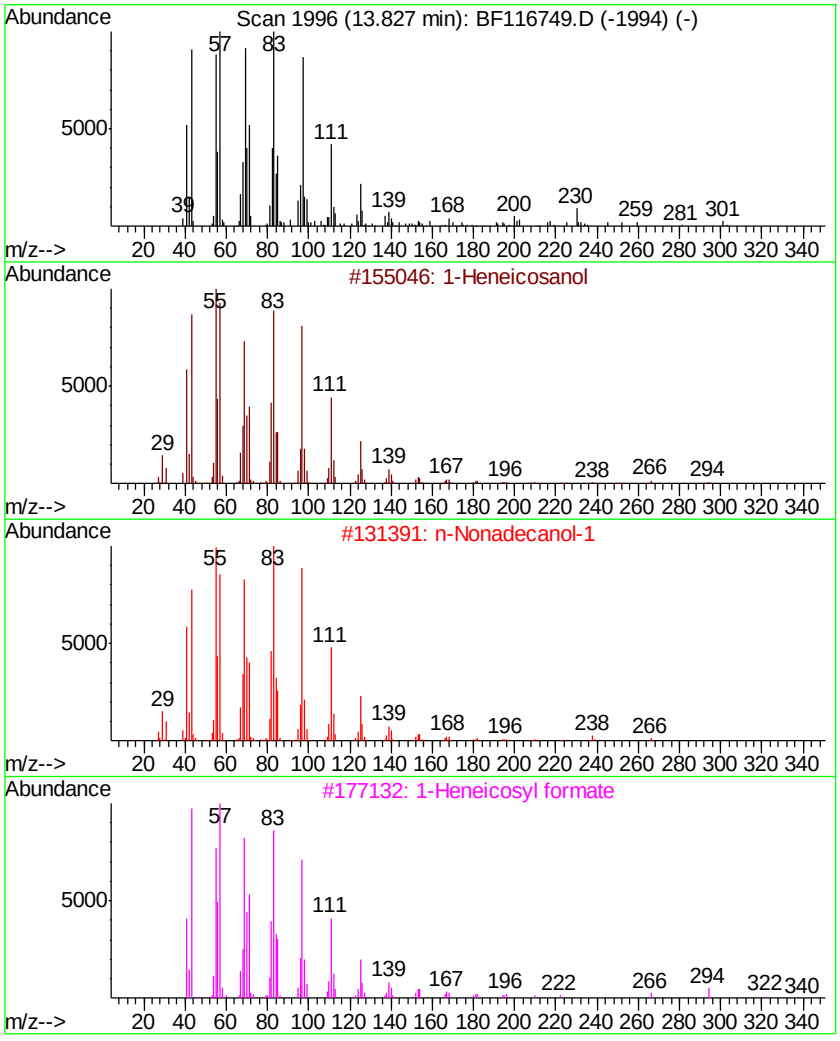
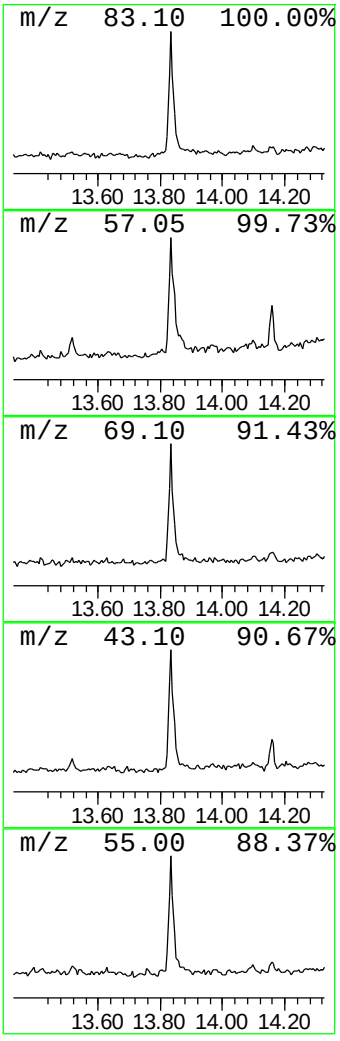
Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.13 ng	351128	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116749.D
Acq On : 1 Sep 2019 18:15
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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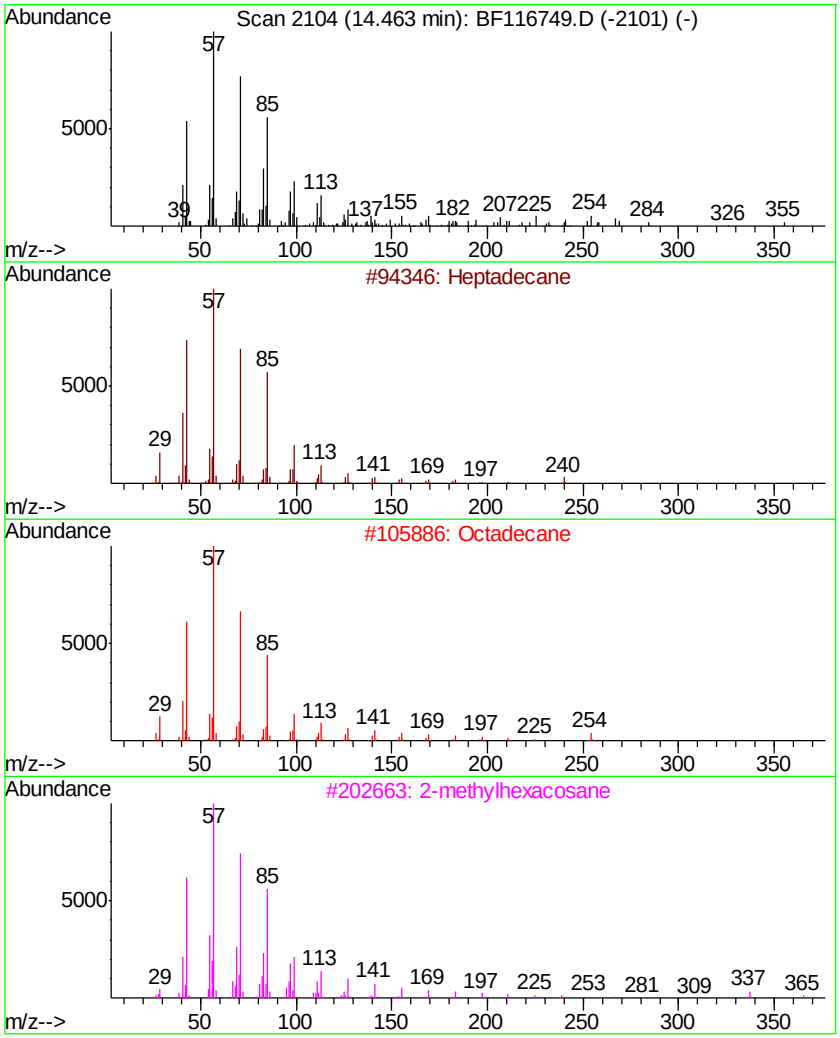
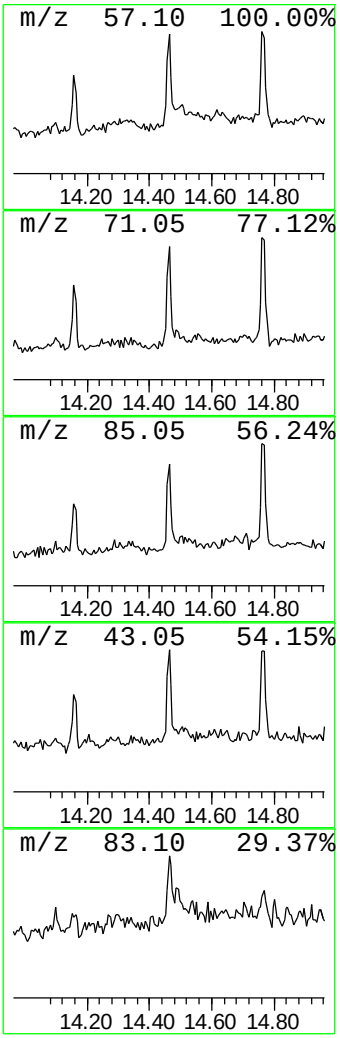
Peak Number 4 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.74 ng	105254	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Octadecane	254	C18H38	000593-45-3	89
3	2-methylhexacosane	380	C27H56	1000376-72-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Tridecane	184	C13H28	000629-50-5	86





Library Search Compound Report

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Data File : BF116749.D
Acq On : 1 Sep 2019 18:15
Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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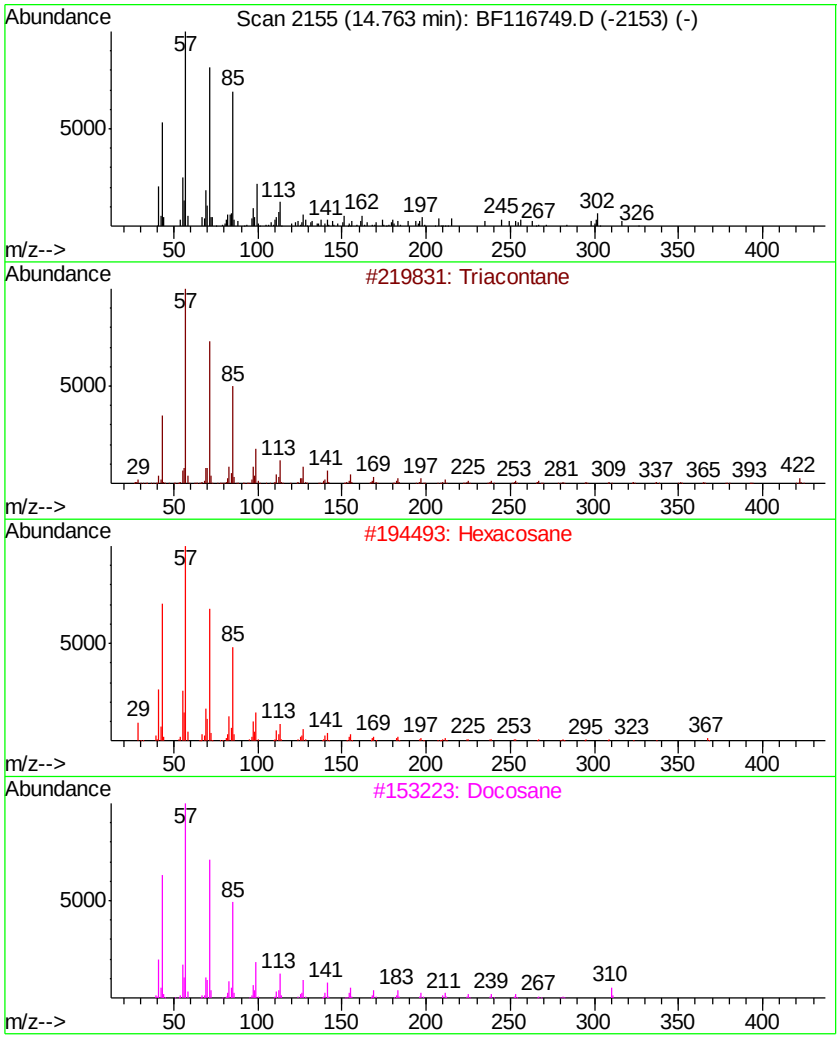
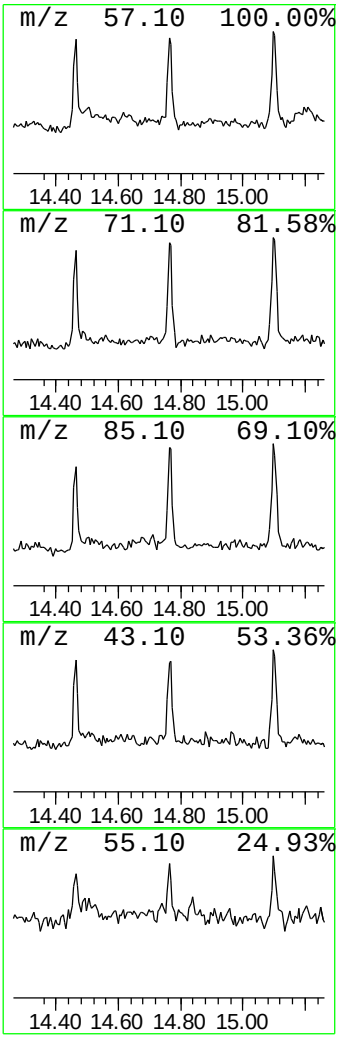
Peak Number 5 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.49 ng	86744	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	86
2	Hexacosane	366	C26H54	000630-01-3	80
3	Docosane	310	C22H46	000629-97-0	78
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	78
5	Nonadecane	268	C19H40	000629-92-5	72





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Operator : HP/JU
Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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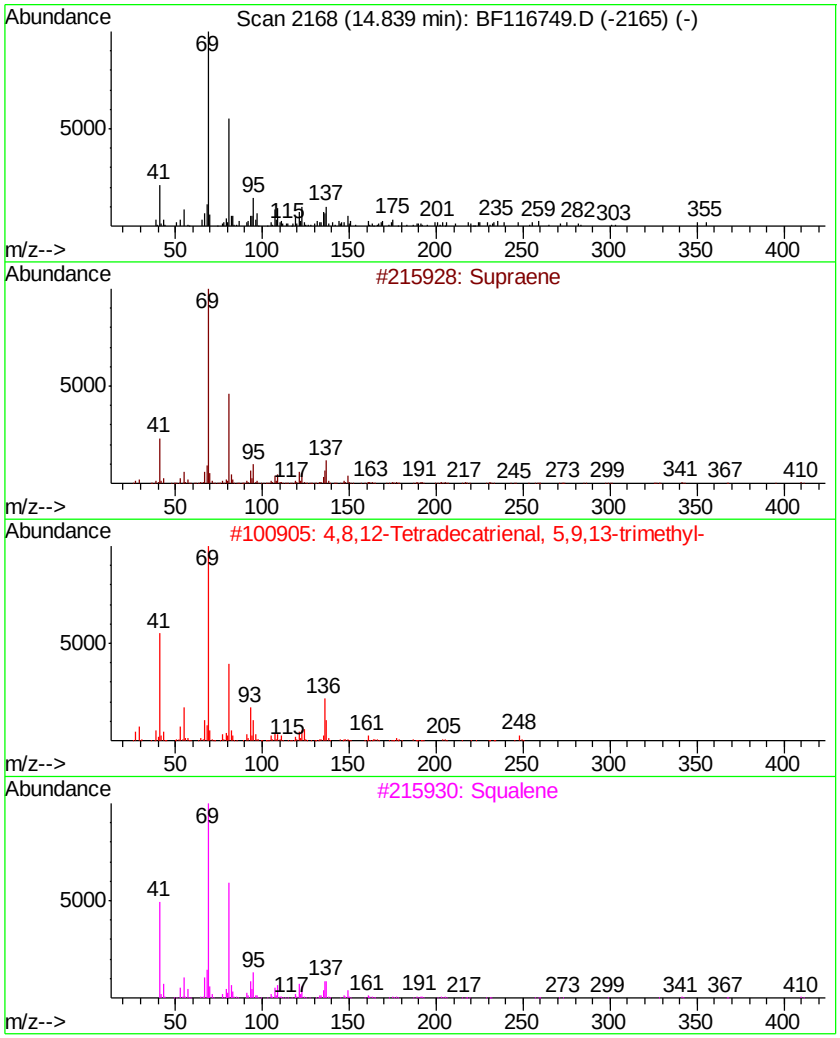
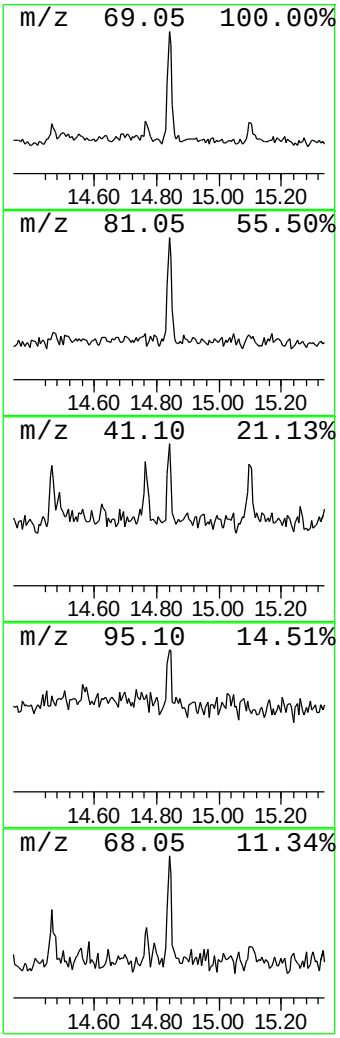
Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.58 ng	89852	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3	Squalene	410	C30H50	000111-02-4	72
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Library Search Compound Report

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Sample : K4548-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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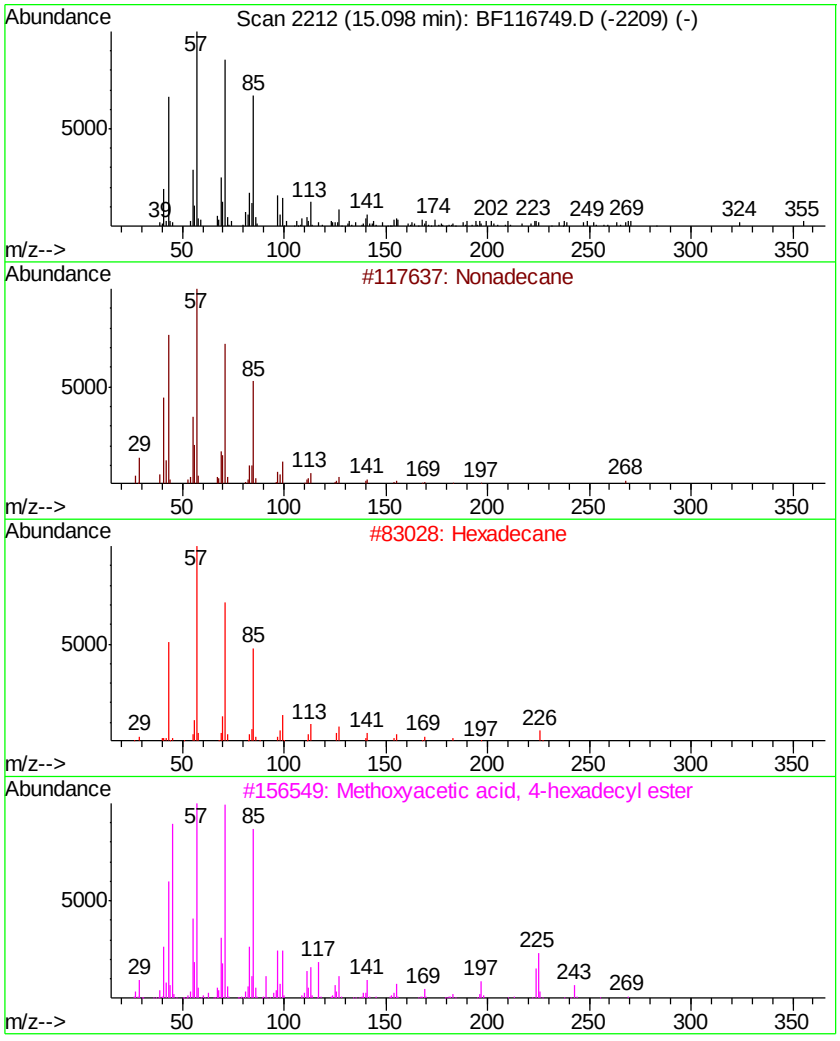
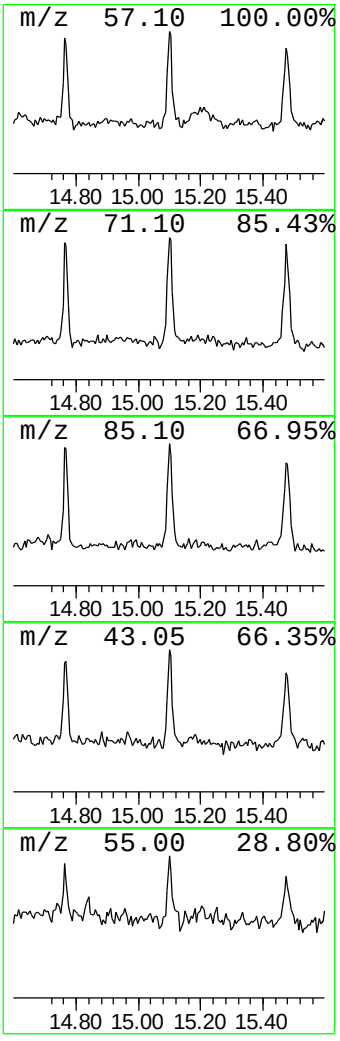
Peak Number 7 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	2.89 ng	100374	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





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Sample : K4548-09
Misc :
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Instrument : BNA_F
ClientSampleId : T8-S-G1-G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

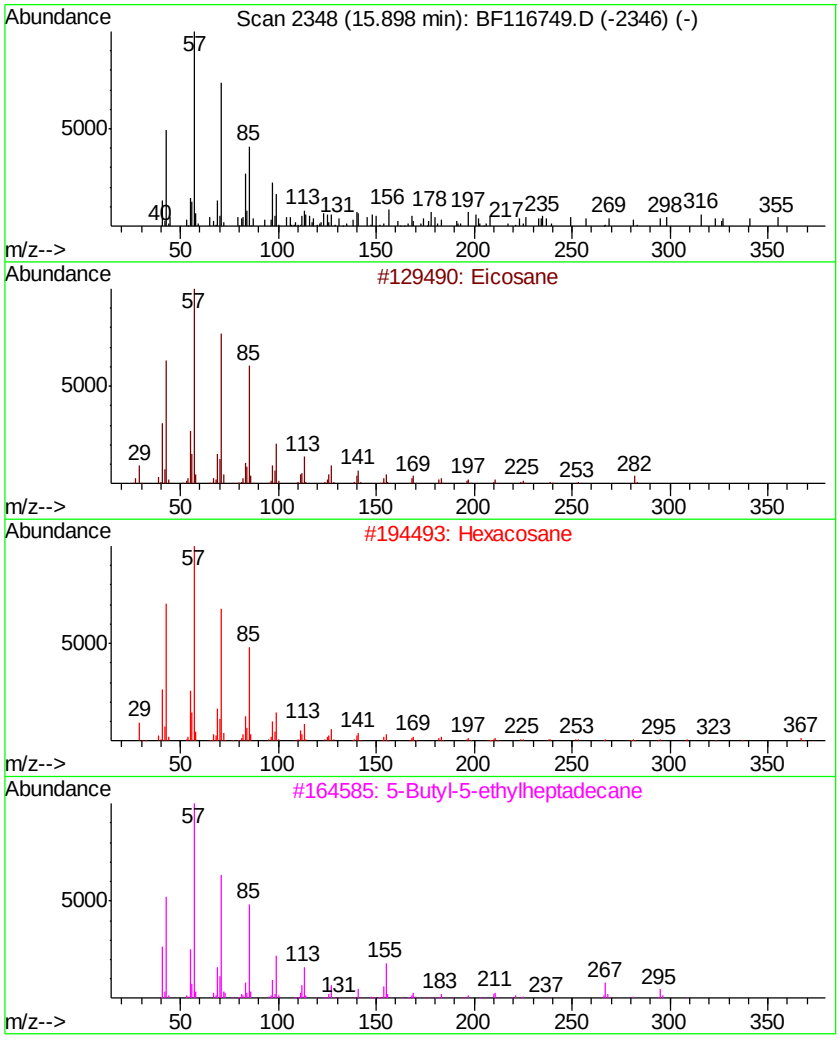
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

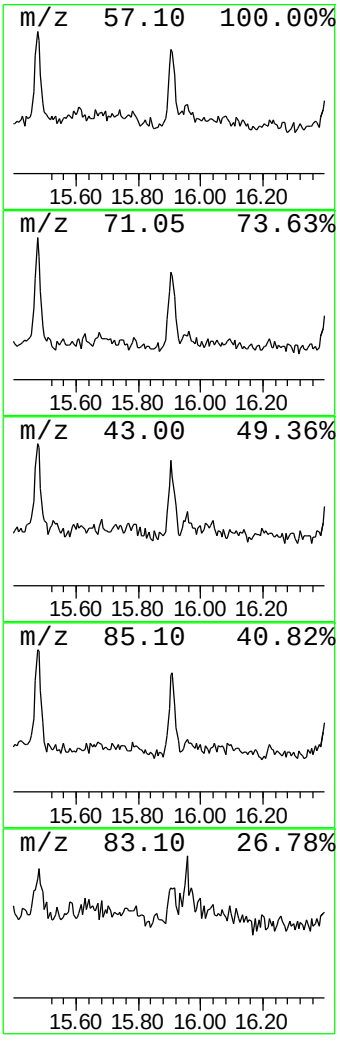
****

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.57 ng	89537	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	83
3	5-Butyl-5-ethylheptadecane	324	C23H48	1000360-43-0	80
4	2-methyloctacosane	408	C29H60	1000376-72-8	80
5	Octacosane	394	C28H58	000630-02-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090119\
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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
unknown6.61	6.61	71.7	ng	1550890	1	6.85	432714	20.0
1-Heneicosanol	13.83	9.1	ng	351128	5	13.99	769177	20.0
Heptadecane	14.46	2.7	ng	105254	5	13.99	769177	20.0
Triacontane	14.76	2.5	ng	86744	6	15.44	695662	20.0
Supraene	14.84	2.6	ng	89852	6	15.44	695662	20.0
Nonadecane	15.10	2.9	ng	100374	6	15.44	695662	20.0
Eicosane	15.90	2.6	ng	89537	6	15.44	695662	20.0