LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113577.D
Acq On : 4 Apr 2019 8:12
Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RICH-REC-ROAD-STONE-14

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-BF040319.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	3.204	185	190	199	rBV2	9127	21601	1.04%	0.103%
2	4.204	355	360	368	rBV	970752	1247561	59.98%	5.959%
3	4.863	467	472	486	rBV	995228	1150326	55.30%	5.495%
4	5.298	543	546	574	rBV	1139899	1266728	60.90%	6.051%
5	6.334	718	722	739	rBV	1588439	1582781	76.09%	7.560%
6	6.457	739	743	754	rVB	1655330	1446390	69.54%	6.909%
7	6.686	778	782	791	rBV	708551	599018	28.80%	2.861%
8	6.757	791	794	803	rVB	19266	23328	1.12%	0.111%
9	6.839	805	808	825	rVB	1475419	1363309	65.54%	6.512%
10	7.245	874	877	889	rBV	946571	966611	46.47%	4.617%
11	7.334	889	892	898	rVB	59690	59525	2.86%	0.284%
12	7.463	911	914	918	rVB	32958	27718	1.33%	0.132%
13	7.504	918	921	926	rBV	28227	27728	1.33%	0.132%
14	7.969	996	1000	1006	rBV	765963	672788	32.34%	3.214%
15	9.045	1179	1183	1195	rBV	2133283	1805193	86.79%	8.623%
16	9.445	1247	1251	1255	rBV	61719	61467	2.96%	0.294%
17	9.722	1294	1298	1312	rVB2	815712	702177	33.76%	3.354%
18	10.510	1429	1432	1444	rBV	498381	514261	24.72%	2.456%
19	10.633	1450	1453	1460	rVB3	23416	36738	1.77%	0.175%
20	10.727	1466	1469	1473	rBV	52852	44548	2.14%	0.213%
21	11.204	1547	1550	1553	rBV	852660	751004	36.10%	3.587%
22	11.269	1558	1561	1568	rVB3	16103	27657	1.33%	0.132%
23	11.510	1599	1602	1606	rVB	25725	25369	1.22%	0.121%
24	11.745	1638	1642	1644	rBV4	15928	24304	1.17%	0.116%
25	11.916	1668	1671	1674	rVB	36196	29738	1.43%	0.142%
26	12.039	1690	1692	1696	rBV5	16279	21972	1.06%	0.105%
27	12.257	1727	1729	1732	rBV3	20132	26772	1.29%	0.128%
28	12.304	1734	1737	1740	rVB	52534	50630	2.43%	0.242%
29	12.416	1753	1756	1759	rBV	63575	69846	3.36%	0.334%
30	12.645	1792	1795	1797	rBV2	63151	57718	2.77%	0.276%
31	12.674	1797	1800	1802	rVV	58254	49477	2.38%	0.236%
32	12.792	1815	1820	1823	rBV	2066522	2080063	100.00%	9.936%
33	13.027	1858	1860	1863	rVB	74888	56806	2.73%	0.271%
34	13.368	1916	1918	1921	rVB	106177	90666	4.36%	0.433%

LSC Area Percent Report

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Acq On : 4 Apr 2019 8:12
Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RICH-REC-ROAD-STONE-14

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-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.698	1971	1974	1984	rVB	227874	335343	16.12%	1.602%
36	13.845	1993	1999	2002	rBV2	733581	924695	44.46%	4.417%
37	14.010	2025	2027	2030	rBV	128915	121521	5.84%	0.580%
38	14.315	2077	2079	2083	rBV	161588	138807	6.67%	0.663%
39	14.610	2127	2129	2133	rBV	201885	229765	11.05%	1.098%
40	14.680	2138	2141	2145	rVB	186006	197991	9.52%	0.946%
41	14.927	2180	2183	2186	rVB	205973	227320	10.93%	1.086%
42	15.257	2236	2239	2246	rVB2	453159	713019	34.28%	3.406%
43	16.068	2373	2377	2385	rBV3	283607	723482	34.78%	3.456%
44	16.292	2412	2415	2423	rVB	221775	341170	16.40%	1.630%

Sum of corrected areas: 20934931

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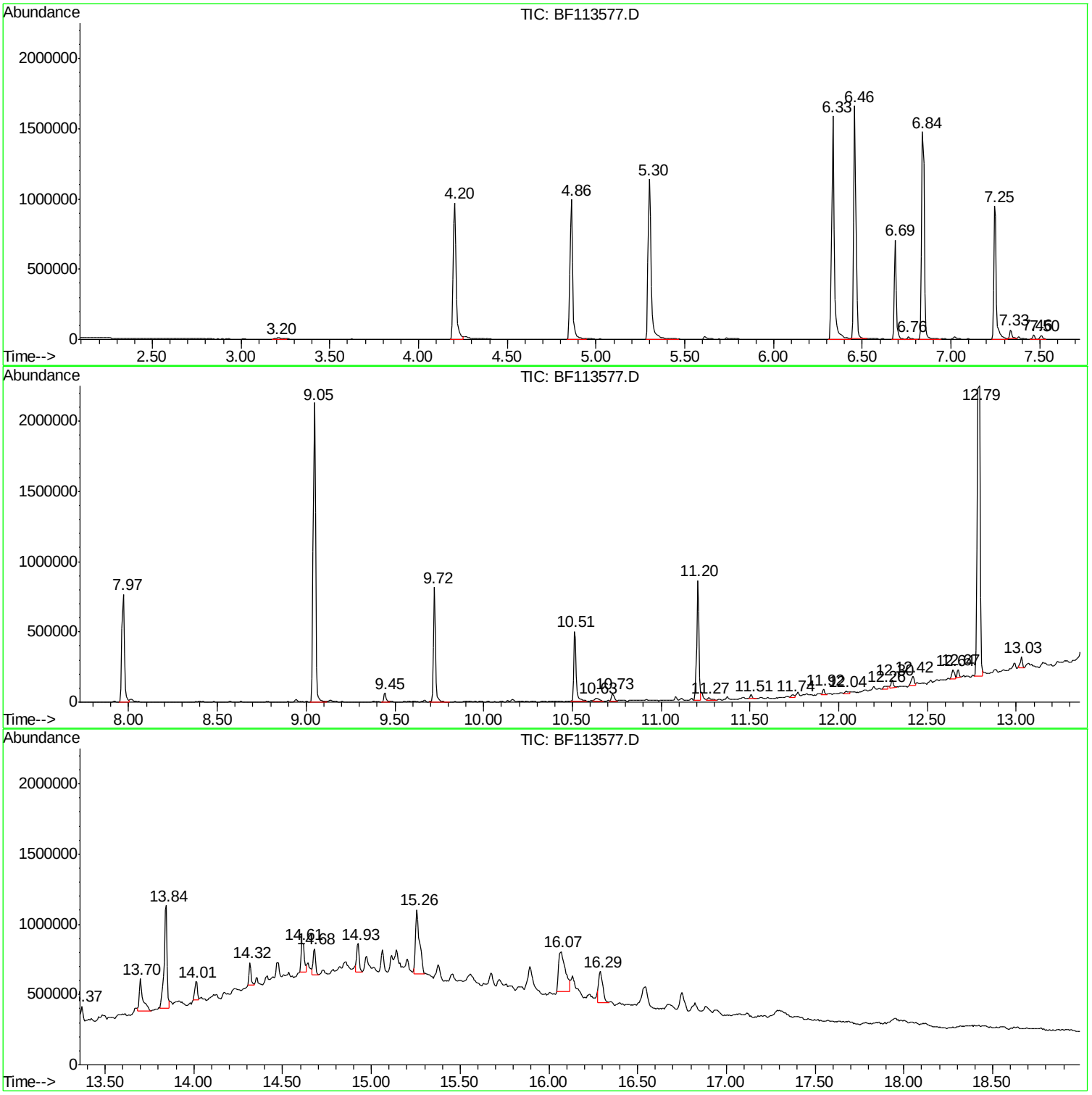
ClientSampleId :
RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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

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Operator : JU/SJ
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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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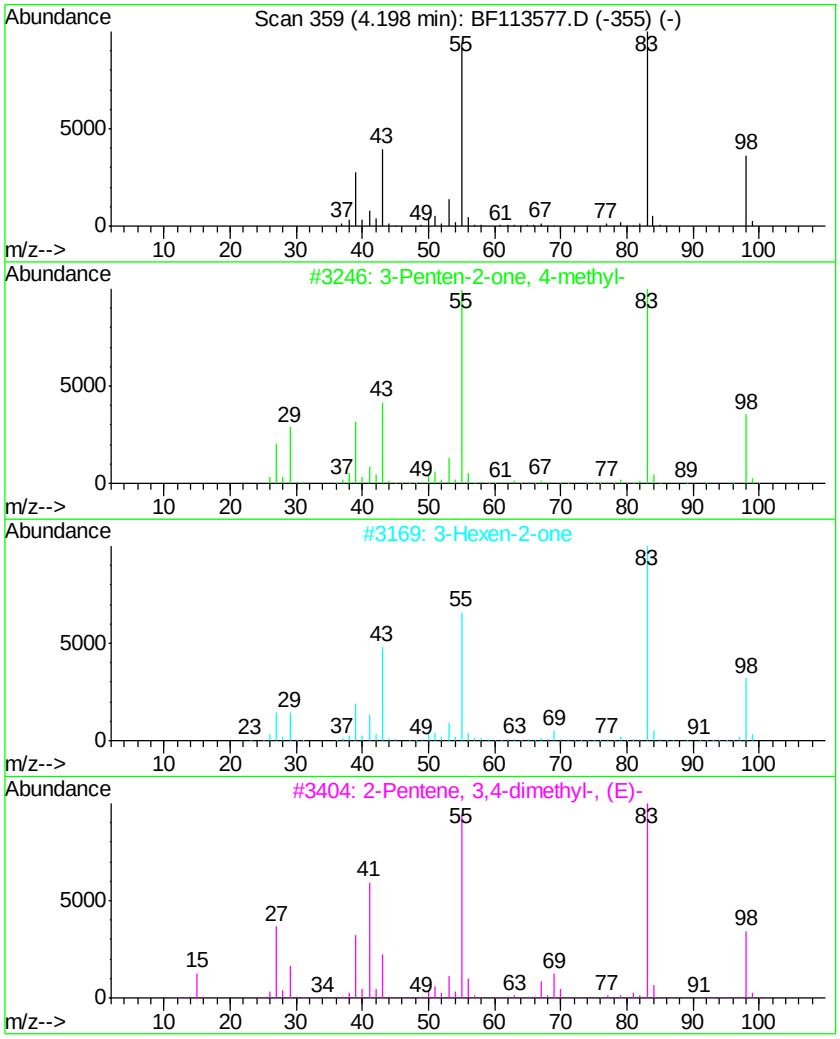
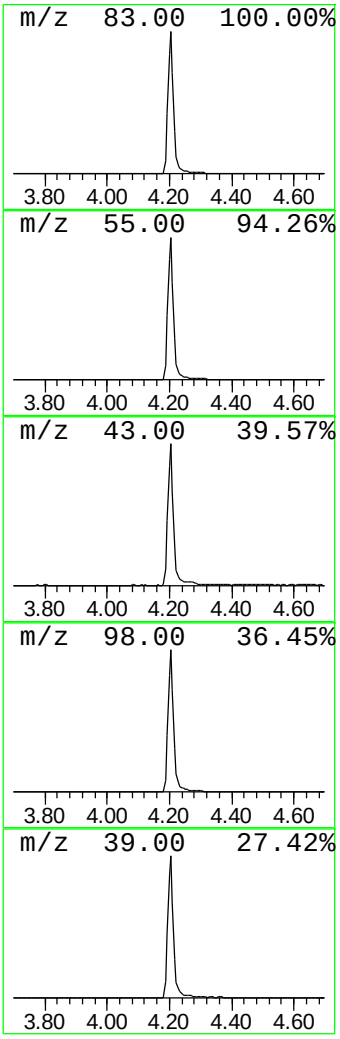
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	41.65 ng	1247560	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Sample : K2230-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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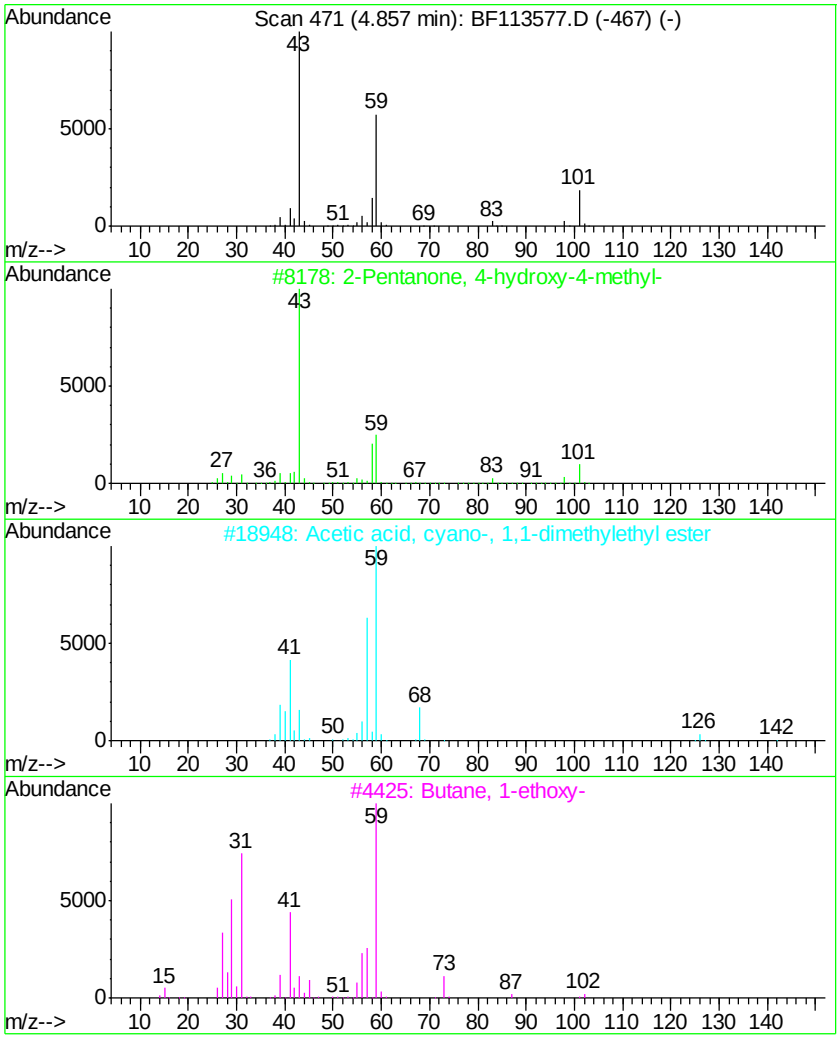
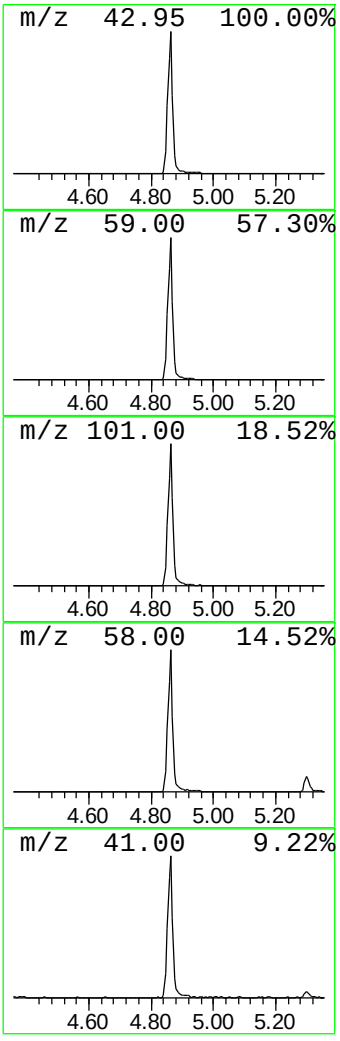
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	38.41 ng	1150330	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113577.D
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Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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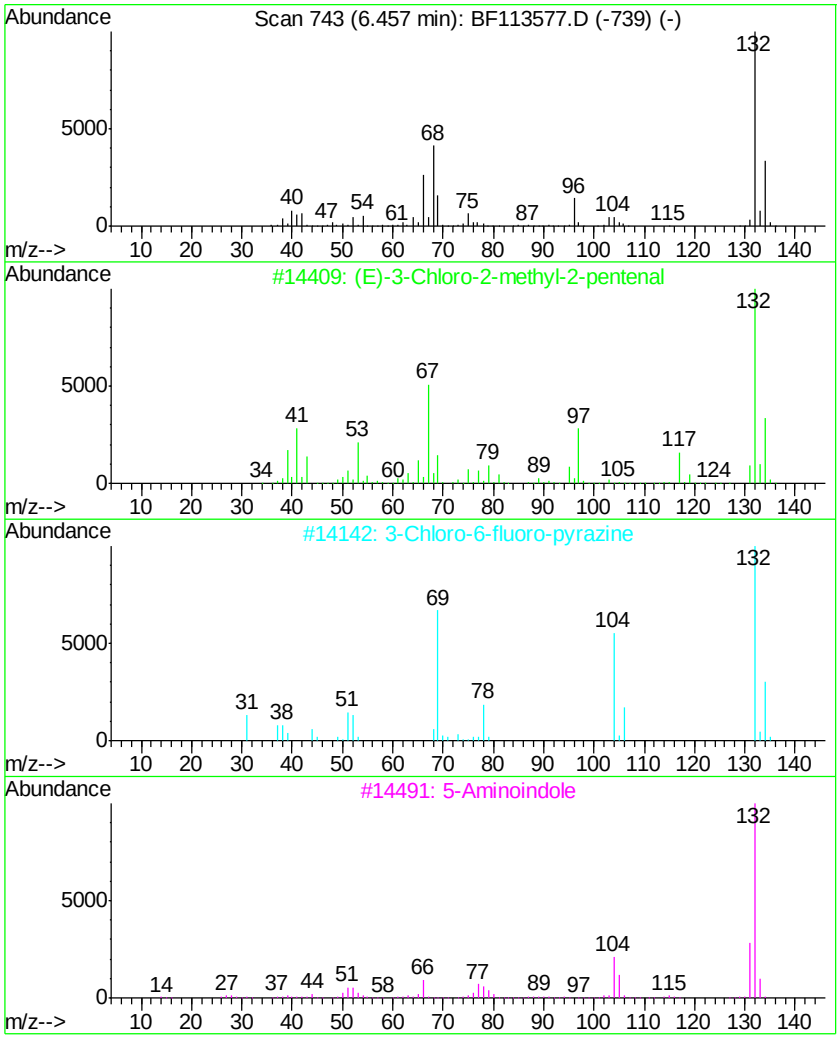
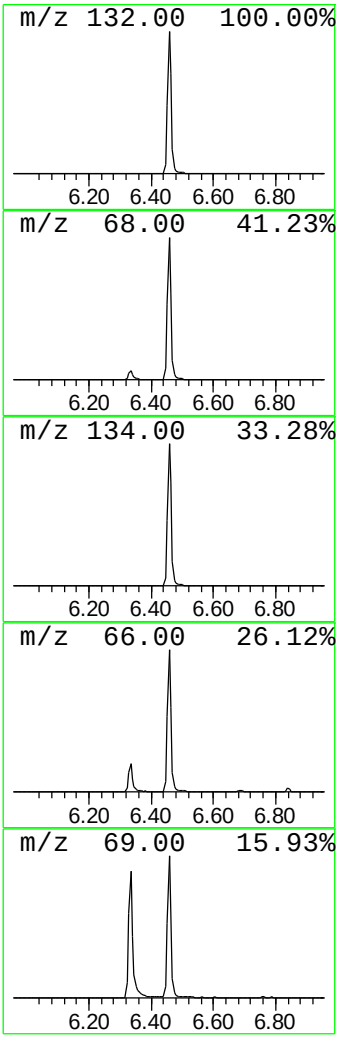
Peak Number 3 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	48.29 ng	1446390	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Library Search Compound Report

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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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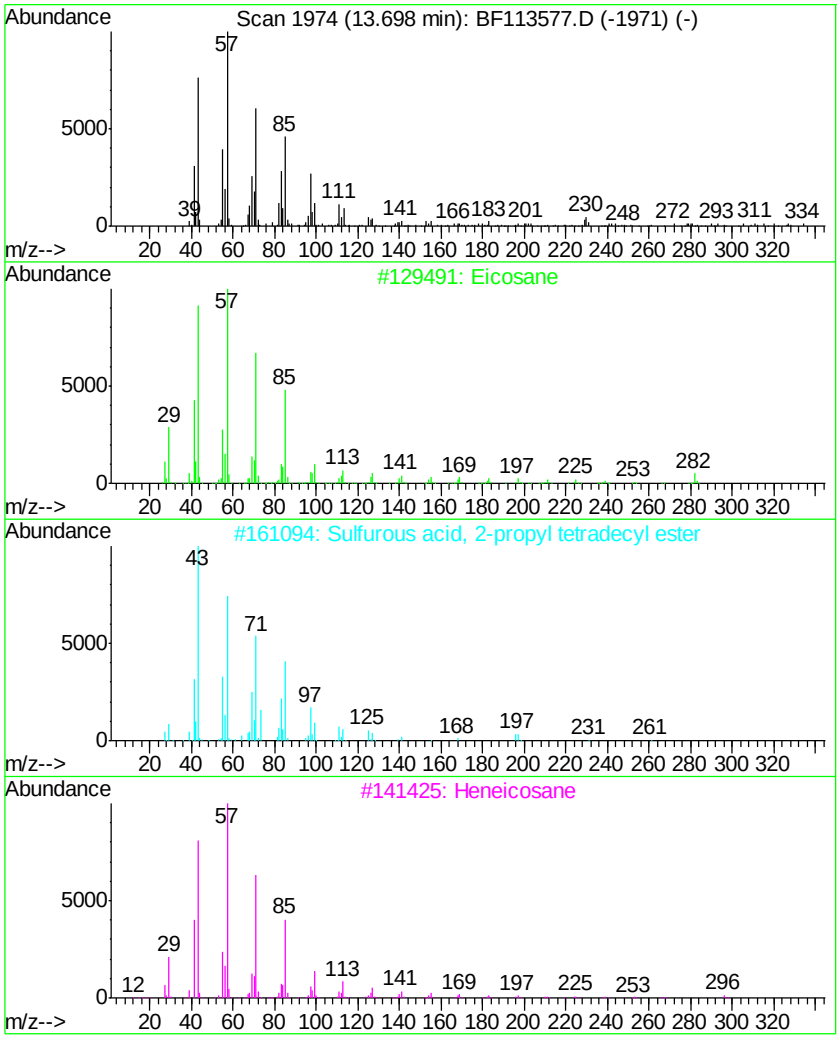
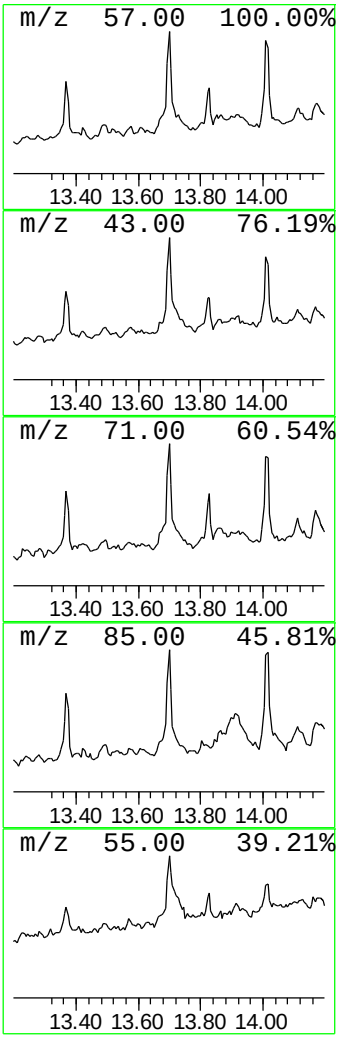
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	7.25 ng	335343	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	83
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	81





Library Search Compound Report

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Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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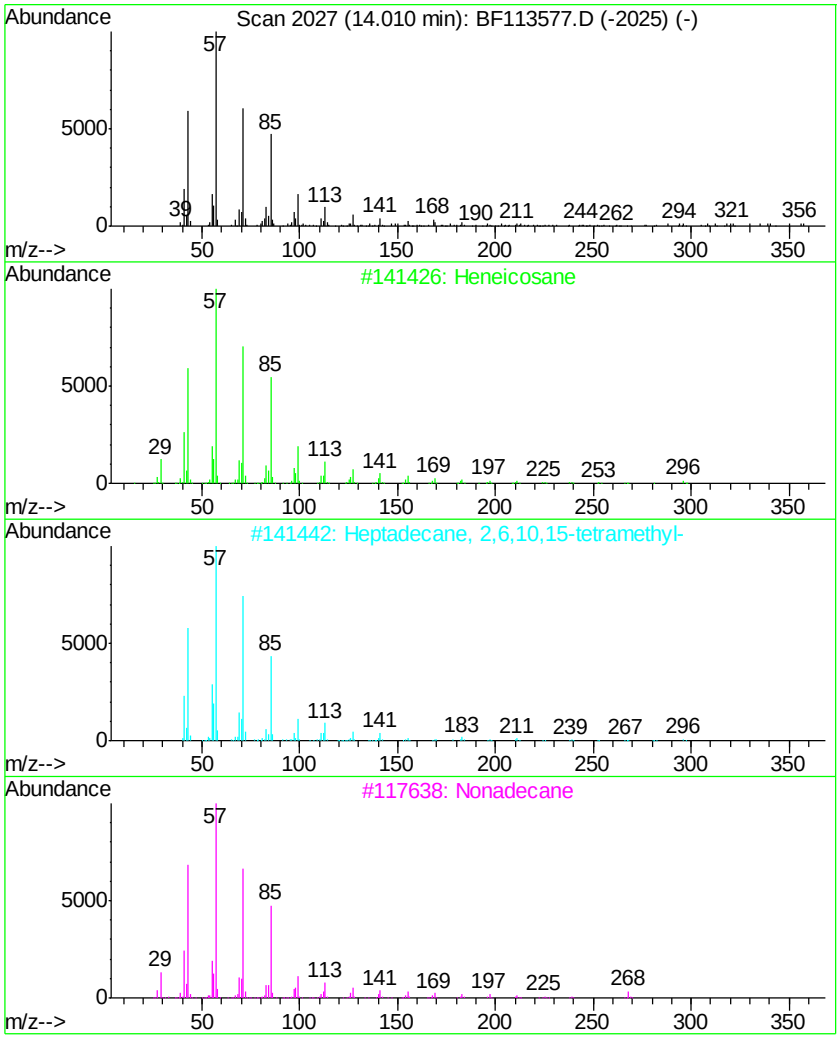
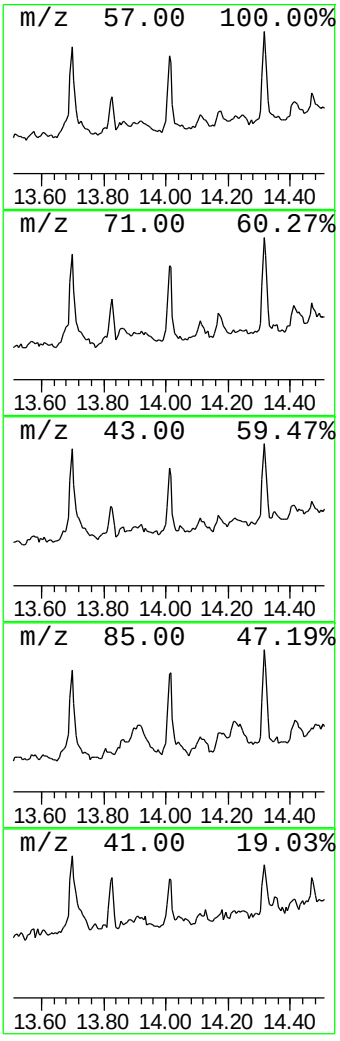
Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.63 ng	121521	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Docosane	310	C22H46	000629-97-0	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
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Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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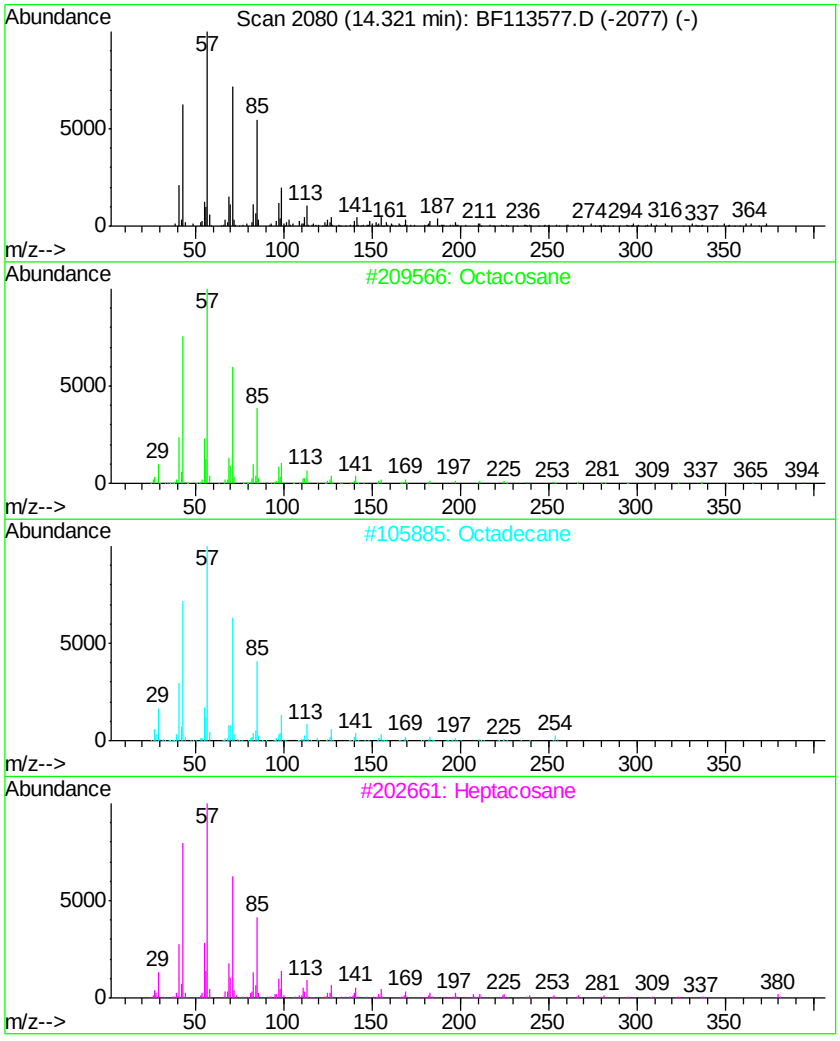
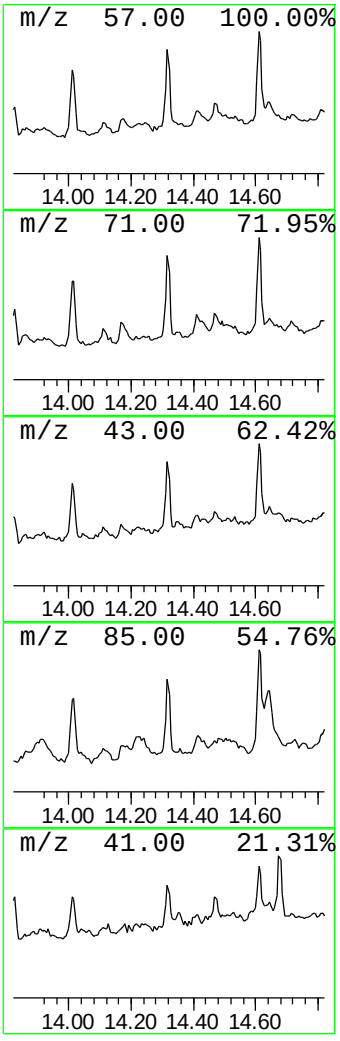
Peak Number 7 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	3.00 ng	138807	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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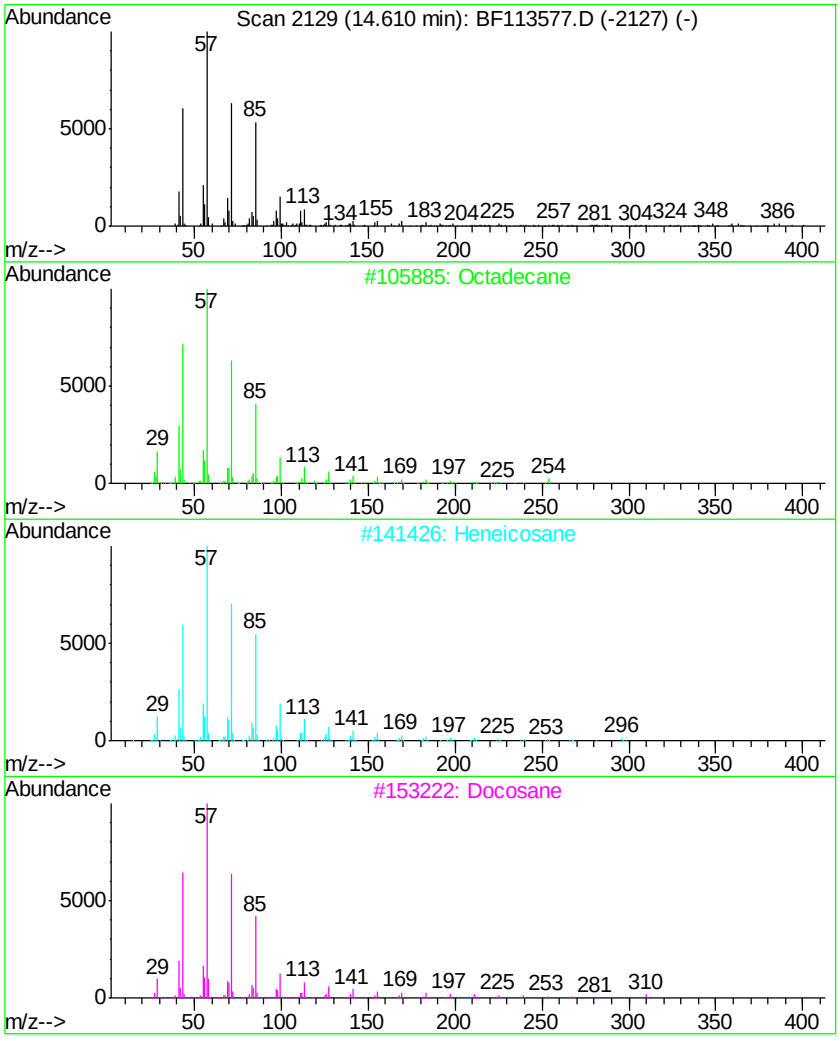
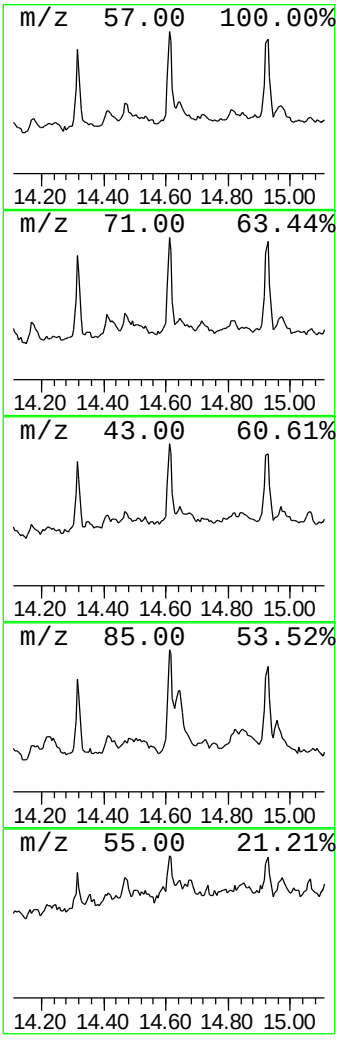
Peak Number 8 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	6.44 ng	229765	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Docosane	310	C22H46	000629-97-0	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Octacosane	394	C28H58	000630-02-4	76





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Acq On : 4 Apr 2019 8:12
Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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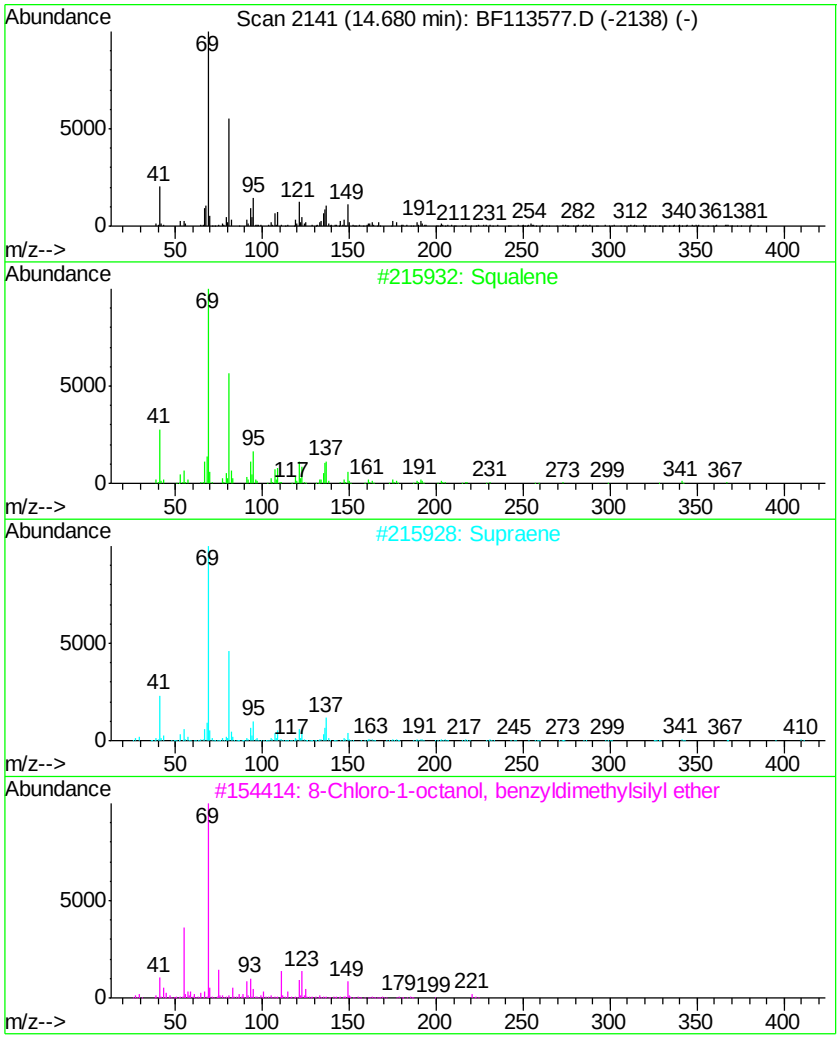
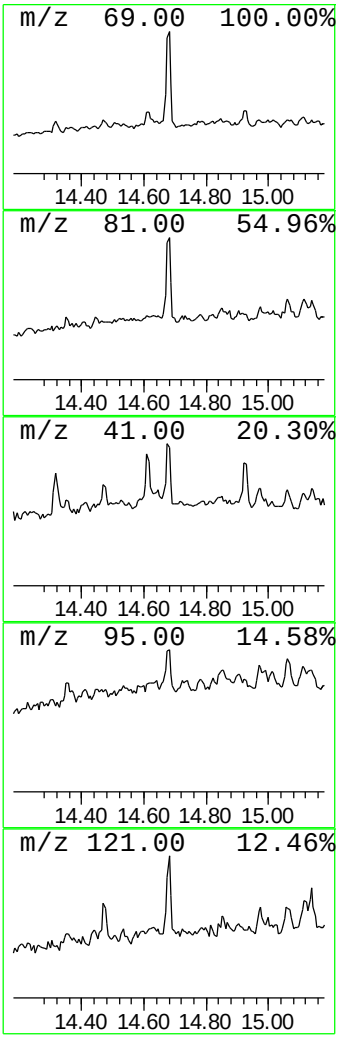
Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	5.55 ng	197991	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	72
3	8-Chloro-1-octanol, benzyldimeth...	312	C17H29ClOSi	1000375-56-9	59
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	45
5	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	45





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Data File : BF113577.D
Acq On : 4 Apr 2019 8:12
Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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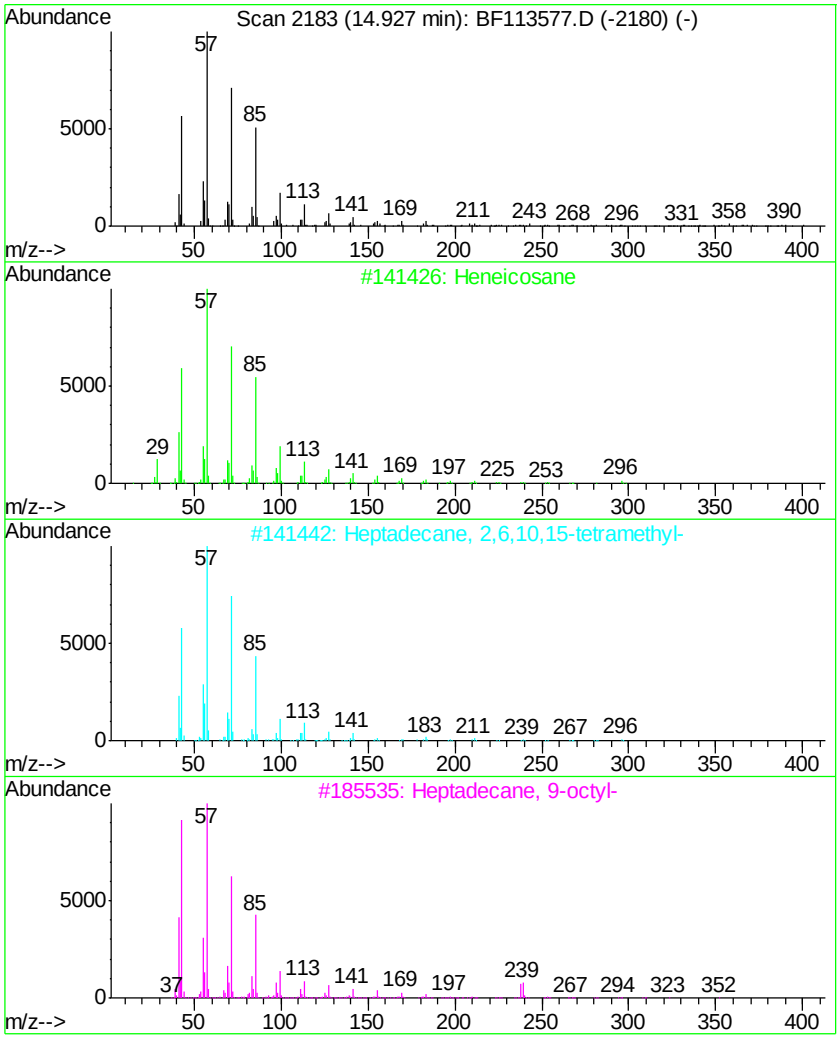
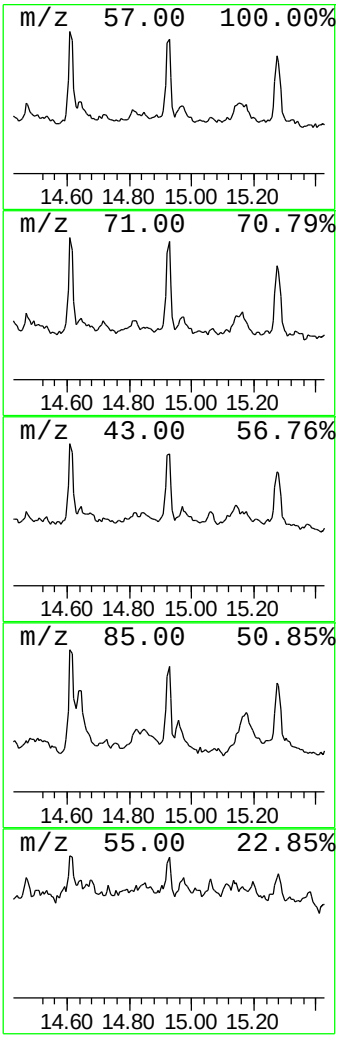
Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	6.38 ng	227320	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	95
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
4	Heptacosane	380	C27H56	000593-49-7	94
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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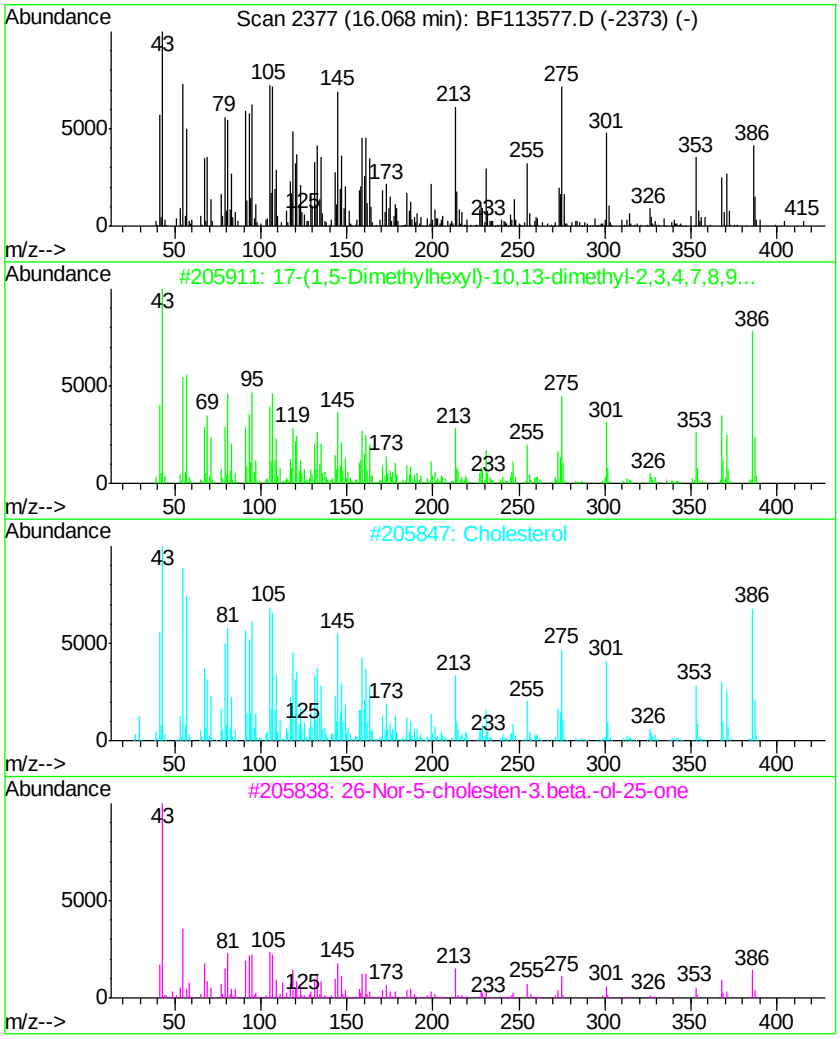
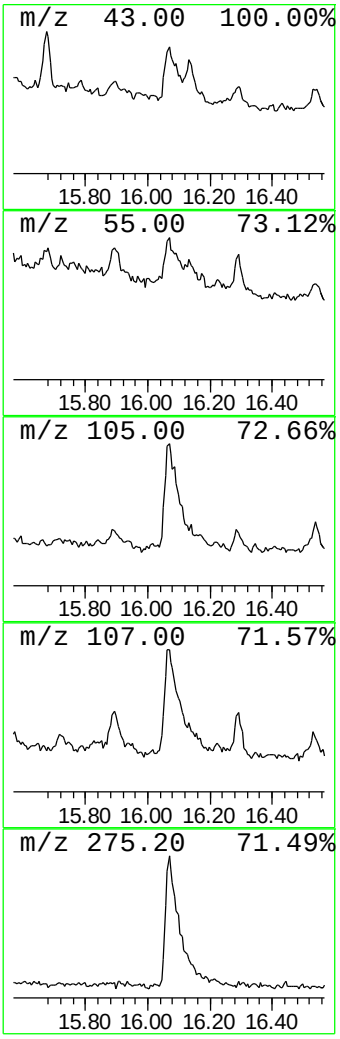
Peak Number 11 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	20.29 ng	723482	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
2	Cholesterol	386	C27H46O	000057-88-5	99
3	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	97
4	Cholesta-3,5-diene	368	C27H44	000747-90-0	25
5	Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	22





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Operator : JU/SJ
Sample : K2230-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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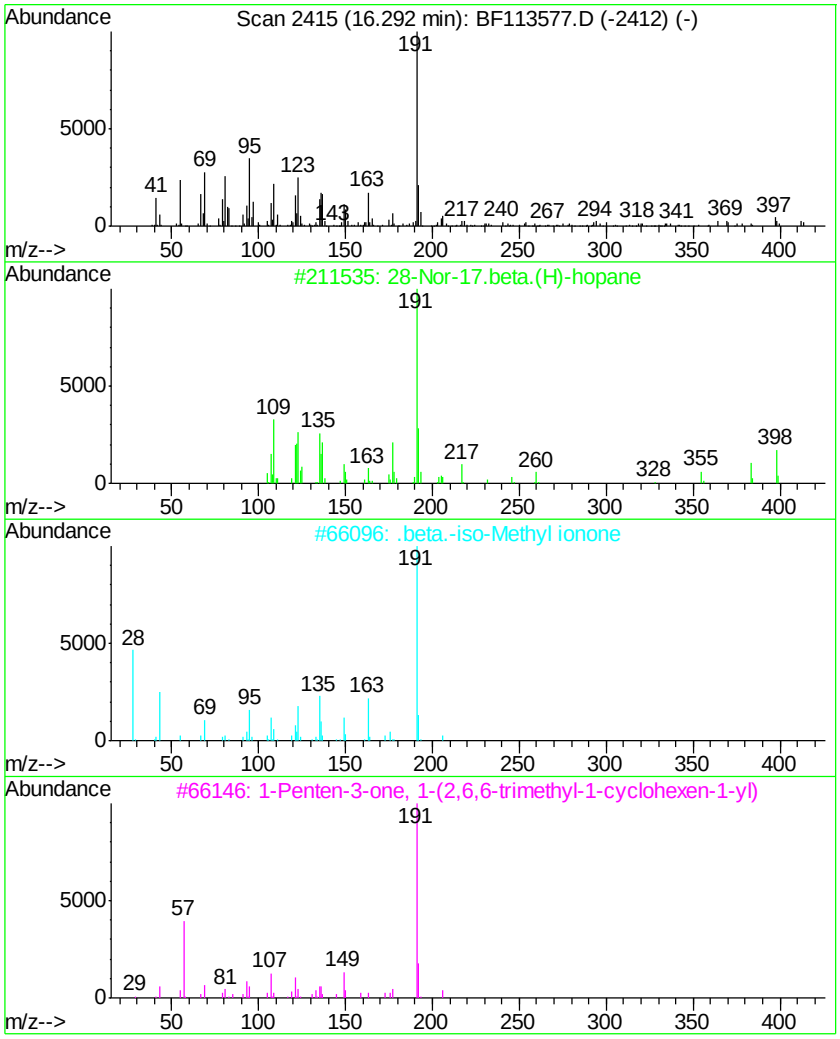
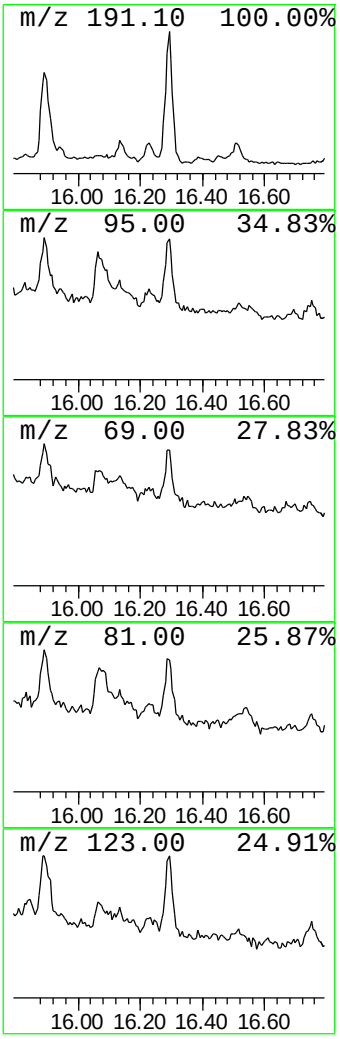
Peak Number 12 28-Nor-17.beta.(H)-hopane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	9.57 ng	341170	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	72
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
4	Isophthalic acid, neopentyl prop...	278	C16H22O4	1000343-85-9	43
5	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	43





Tentatively Identified Compound (LSC) summary

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ClientSampleId : RICH-REC-ROAD-STONE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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
3-Penten-2-one, 4...	4.20	41.6	ng	1247560	1	6.69	599018	20.0
2-Pentanone, 4-hy...	4.86	38.4	ng	1150330	1	6.69	599018	20.0
unknown6.46	6.46	48.3	ng	1446390	1	6.69	599018	20.0
Eicosane	13.70	7.3	ng	335343	5	13.84	924695	20.0
Heptadecane, 2,6,...	14.01	2.6	ng	121521	5	13.84	924695	20.0
Octacosane	14.32	3.0	ng	138807	5	13.84	924695	20.0
Docosane	14.61	6.4	ng	229765	6	15.26	713019	20.0
Squalene	14.68	5.5	ng	197991	6	15.26	713019	20.0
Heneicosane	14.93	6.4	ng	227320	6	15.26	713019	20.0
17-(1,5-Dimethylh...	16.07	20.3	ng	723482	6	15.26	713019	20.0
28-Nor-17.beta.(H...	16.29	9.6	ng	341170	6	15.26	713019	20.0