LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

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-BF092218.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	4.899	475	478	486	rBV	55455	70519	3.80%	0.348%
2	5.316	545	549	552	rBV	1827459	1685770	90.87%	8.317%
3	6.346	719	724	742	rVB	1993598	1824974	98.37%	9.004%
4	6.475	742	746	749	rBV	2126462	1855191	100.00%	9.153%
5	6.704	782	785	789	rBV	855922	675925	36.43%	3.335%
6	6.863	808	812	815	rBV	1757274	1393297	75.10%	6.874%
7	7.263	876	880	883	rBV	1269585	1174943	63.33%	5.797%
8	7.987	999	1003	1006	rBV	1080863	853642	46.01%	4.212%
9	9.063	1182	1186	1189	rBV	2271335	1801899	97.13%	8.890%
10	9.457	1249	1253	1256	rBV	805255	636711	34.32%	3.141%
11	9.734	1296	1300	1304	rBV2	1067603	949339	51.17%	4.684%
12	10.516	1430	1433	1446	rVB	1094649	1082623	58.36%	5.341%
13	10.657	1453	1457	1463	rBV3	30807	34102	1.84%	0.168%
14	10.710	1463	1466	1468	rBV	68485	58051	3.13%	0.286%
15	10.739	1468	1471	1475	rVV2	62702	83334	4.49%	0.411%
16	10.775	1475	1477	1480	rVV2	64320	64249	3.46%	0.317%
17	10.798	1480	1481	1484	rVV	39789	28661	1.54%	0.141%
18	10.845	1484	1489	1490	rVV2	25746	36122	1.95%	0.178%
19	10.886	1493	1496	1500	rVV3	57331	70641	3.81%	0.349%
20	10.922	1500	1502	1505	rVV	57150	58484	3.15%	0.289%
21	10.963	1507	1509	1513	rVB	36257	32923	1.77%	0.162%
22	11.210	1548	1551	1554	rBV	939055	854934	46.08%	4.218%
23	11.233	1554	1555	1558	rVB	85464	48910	2.64%	0.241%
24	11.751	1639	1643	1647	rBV2	65005	68311	3.68%	0.337%
25	12.416	1753	1756	1760	rBV	164693	136799	7.37%	0.675%
26	12.645	1789	1795	1798	rBV	130020	139391	7.51%	0.688%
27	12.680	1798	1801	1808	rVB2	31212	42990	2.32%	0.212%
28	12.792	1816	1820	1823	rBV	1568535	1306750	70.44%	6.447%
29	12.974	1848	1851	1854	rVB	23544	22725	1.22%	0.112%
30	13.039	1856	1862	1865	rBV	25319	28824	1.55%	0.142%
31	13.710	1973	1976	1990	rVB4	79230	159451	8.59%	0.787%
32	13.839	1993	1998	2001	rVV	858834	891996	48.08%	4.401%
33	13.863	2001	2002	2005	rVB	85497	43559	2.35%	0.215%
34	13.945	2011	2016	2020	rBV4	25241	39867	2.15%	0.197%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.021	2026	2029	2032	rBV2	22545	21705	1.17%	0.107%
36	14.321	2076	2080	2083	rBV2	45601	56113	3.02%	0.277%
37	14.474	2103	2106	2111	rBV3	22933	28431	1.53%	0.140%
38	14.616	2127	2130	2134	rVB	53576	53607	2.89%	0.264%
39	14.686	2138	2142	2146	rVV	305426	277747	14.97%	1.370%
40	14.751	2151	2153	2158	rVB3	30686	34509	1.86%	0.170%
41	14.839	2165	2168	2179	rVB	101646	197545	10.65%	0.975%
42	14.933	2181	2184	2188	rVB2	76725	87191	4.70%	0.430%
43	15.121	2213	2216	2222	rVB	60769	82506	4.45%	0.407%
44	15.174	2222	2225	2229	rBV	66088	76220	4.11%	0.376%
45	15.239	2231	2236	2240	rBV	595177	698121	37.63%	3.444%
46	15.286	2240	2244	2247	rVB2	67634	95739	5.16%	0.472%
47	15.686	2308	2312	2317	rBV	72248	90210	4.86%	0.445%
48	16.145	2386	2390	2396	rBV2	43325	76729	4.14%	0.379%
49	16.580	2461	2464	2470	rVB2	23095	39833	2.15%	0.197%
50	16.686	2478	2482	2488	rVB2	27370	49621	2.67%	0.245%
51	16.980	2527	2532	2538	rBV2	21221	46674	2.52%	0.230%

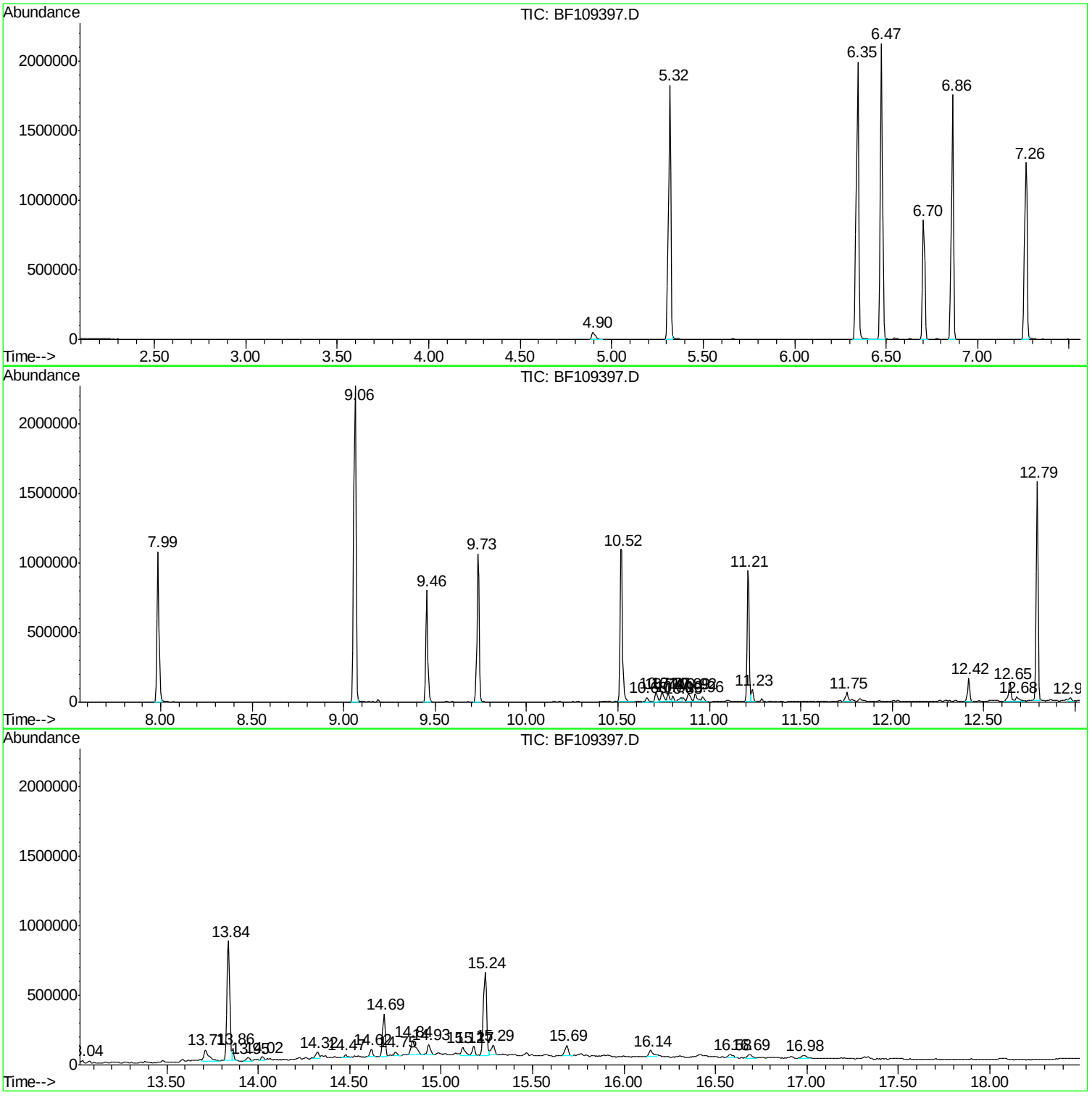
Sum of corrected areas: 20268408

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

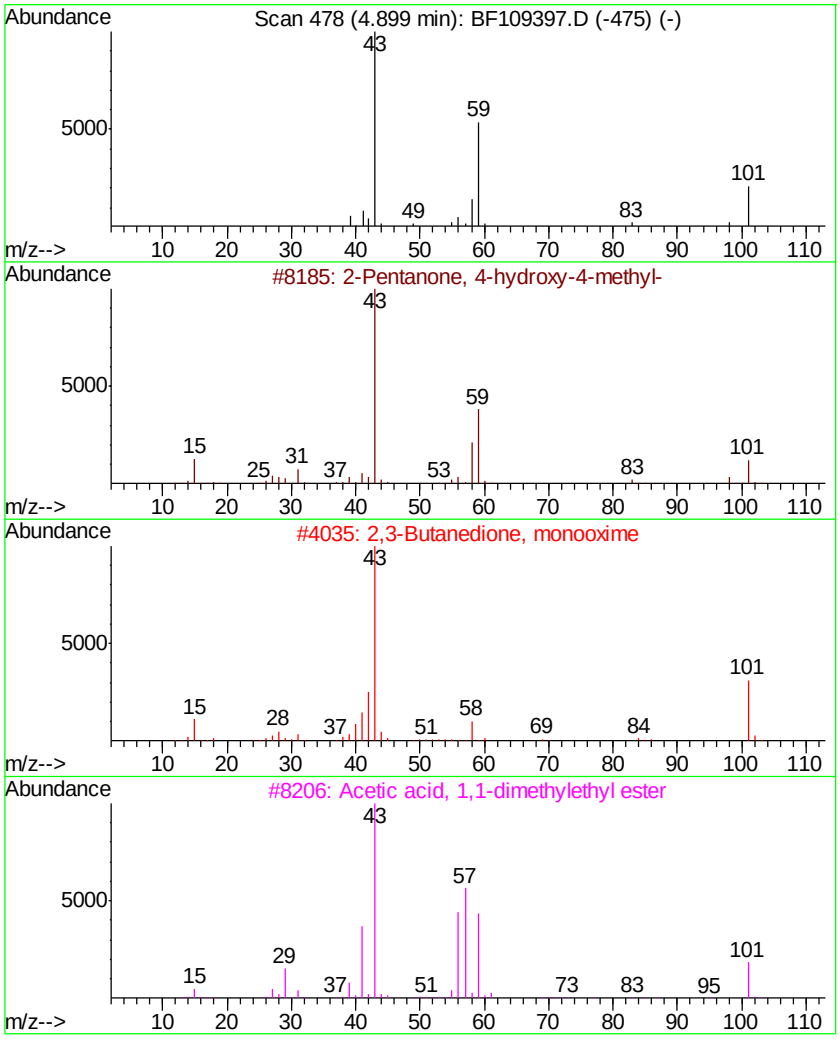
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

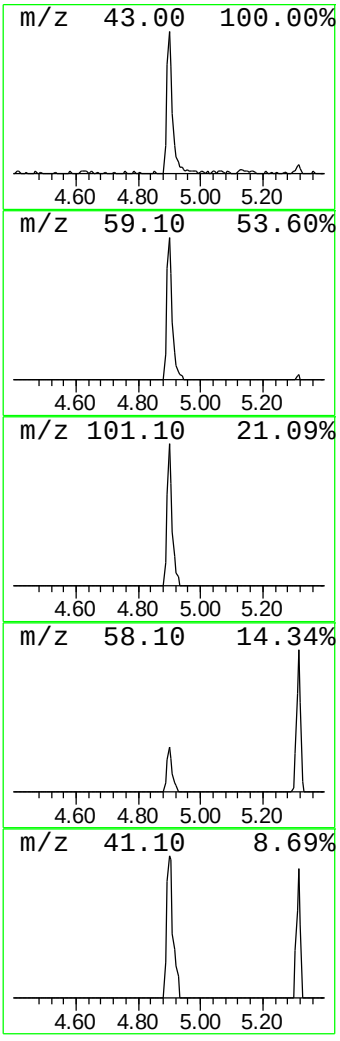
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.09 ng	70519	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

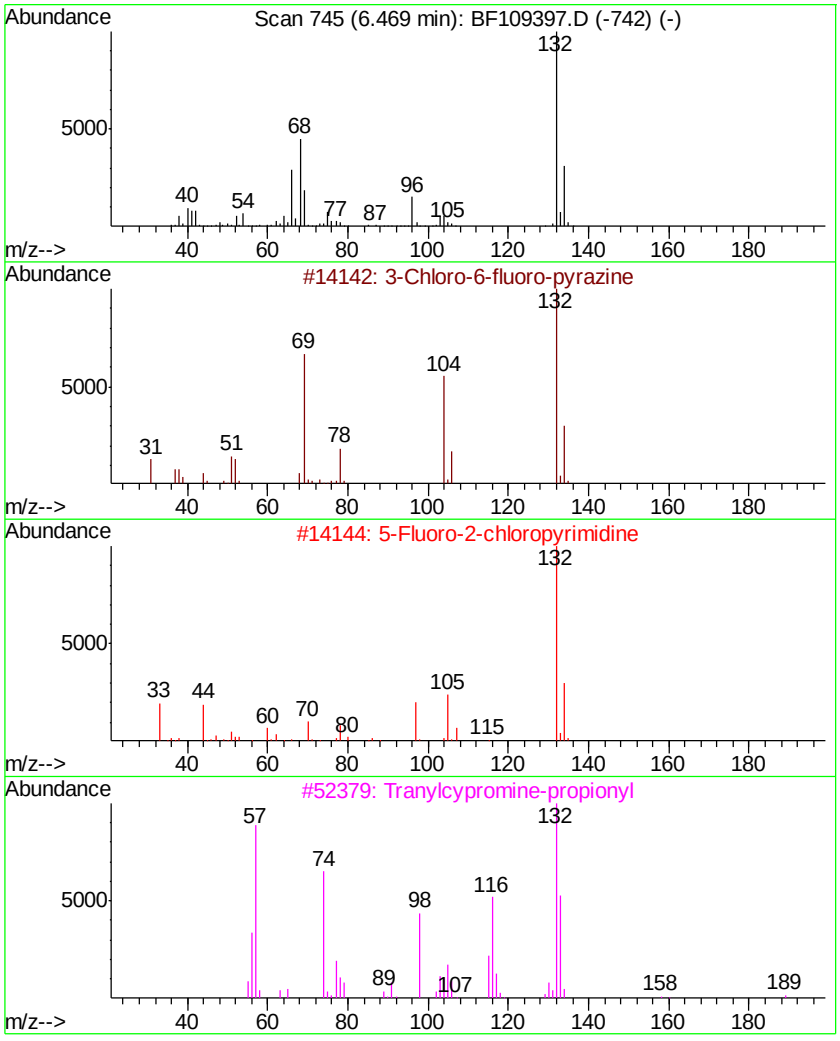
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

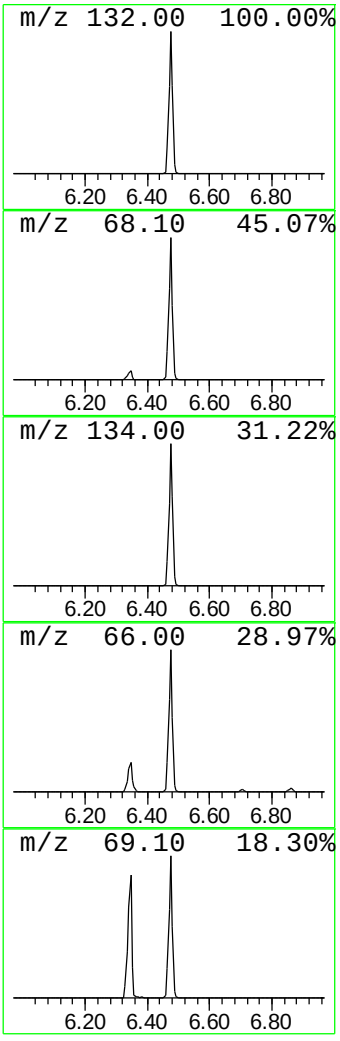
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	54.89 ng	1855190	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

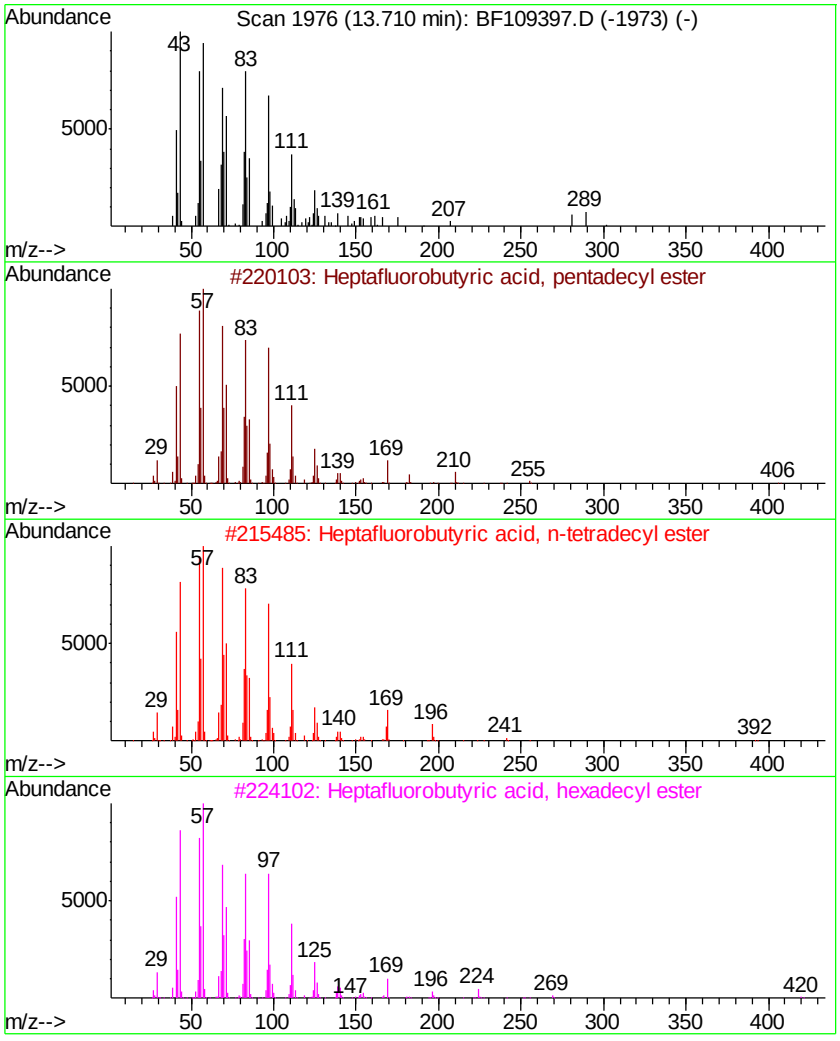
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

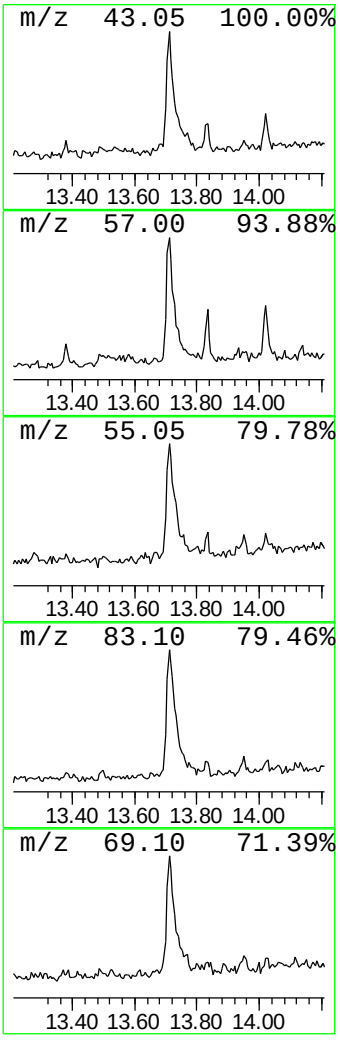
****

Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.58 ng	159451	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

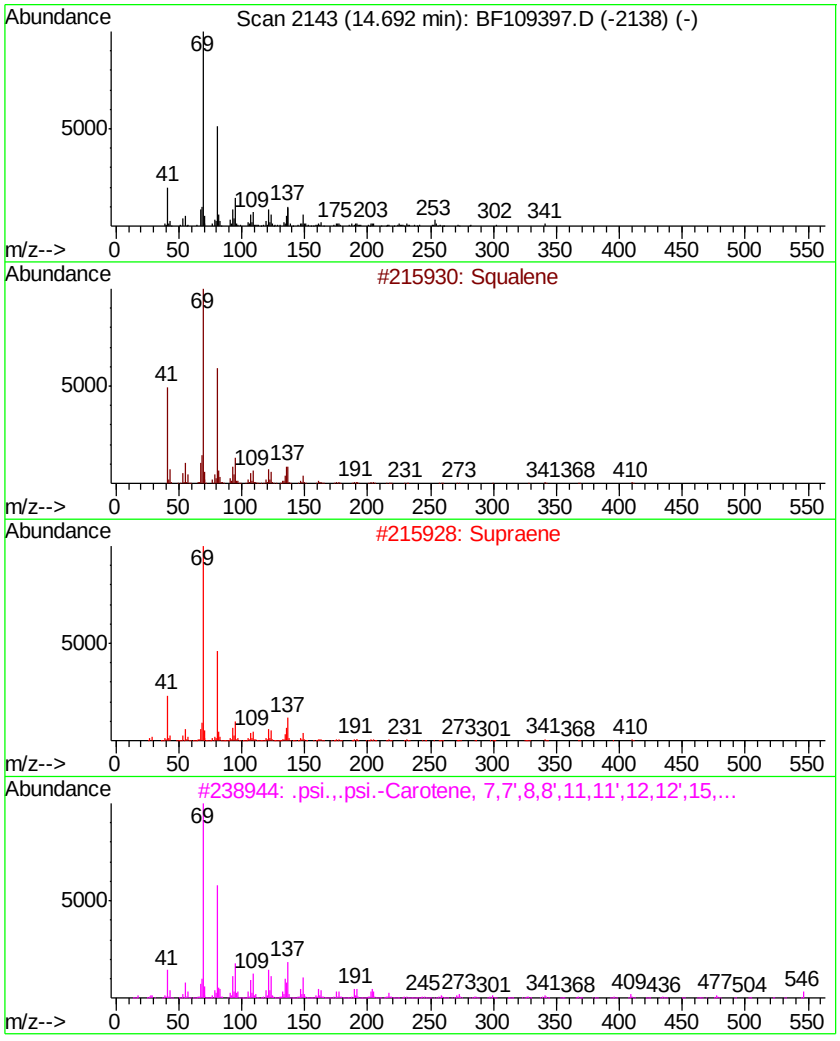
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

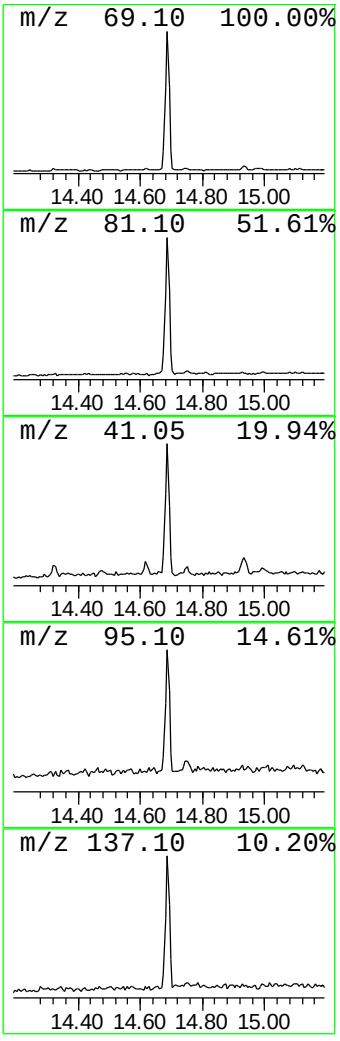
****

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	7.96 ng	277747	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	trans-Farnesol	222	C15H26O	000106-28-5	72
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

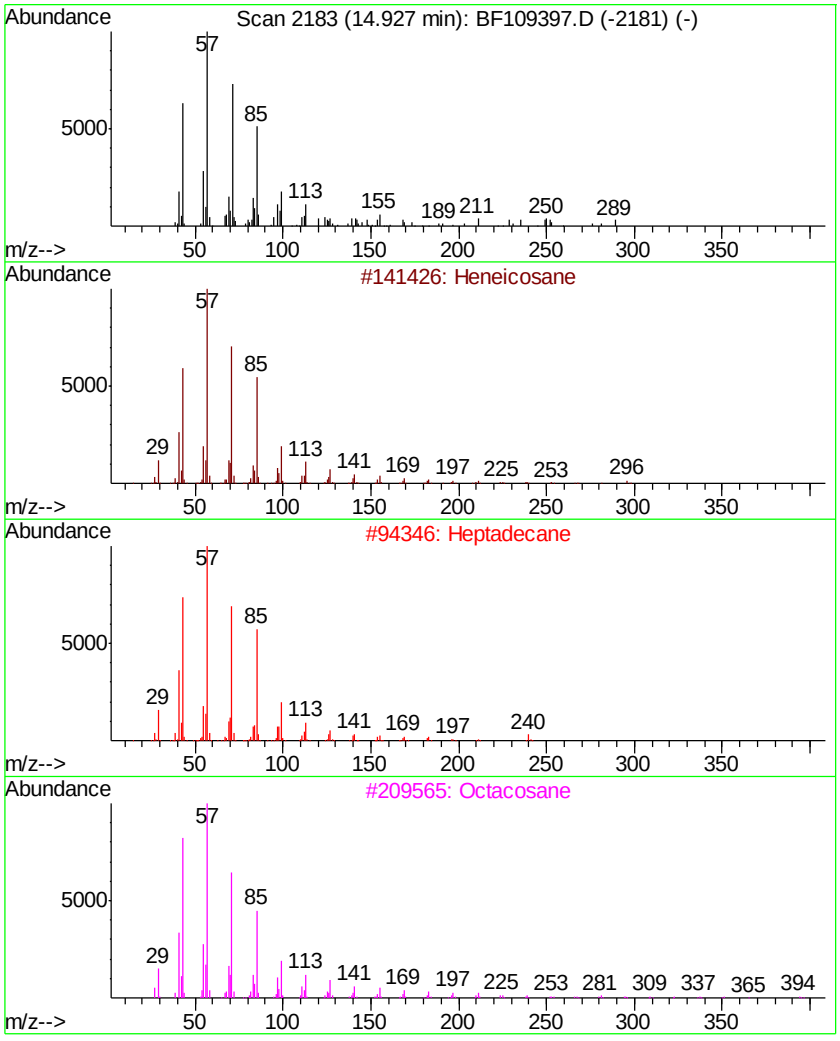
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

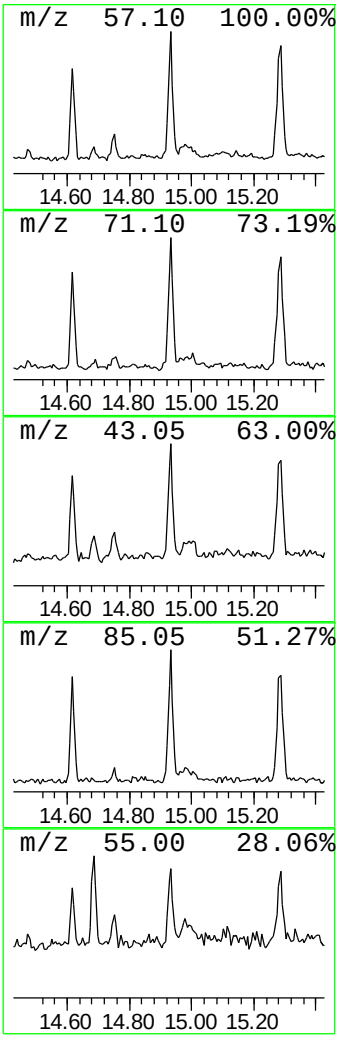
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.50 ng	87191	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane	240	C17H36	000629-78-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

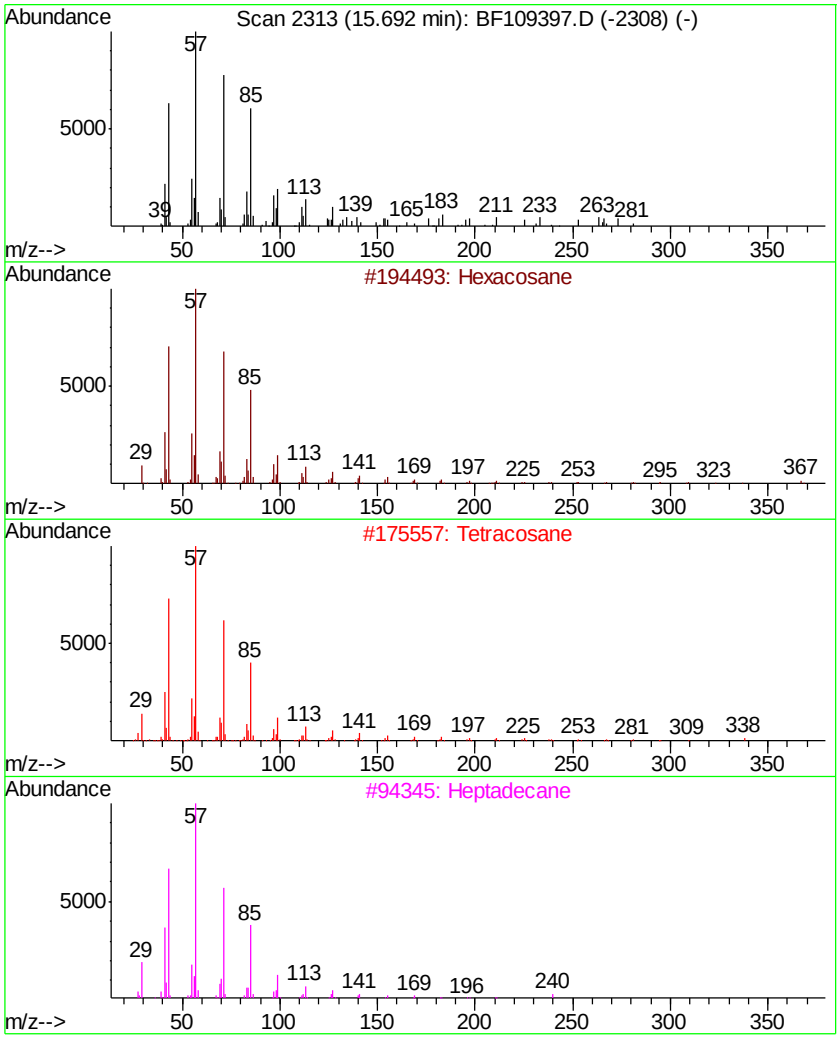
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

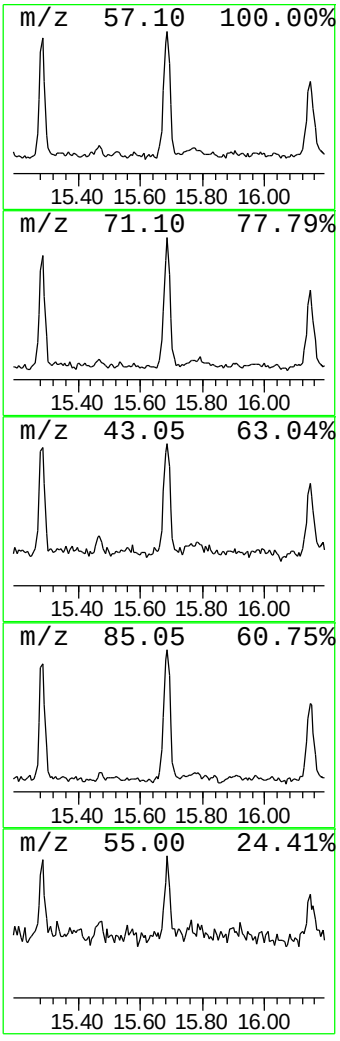
****

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.58 ng	90210	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Heneicosane	296	C21H44	000629-94-7	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

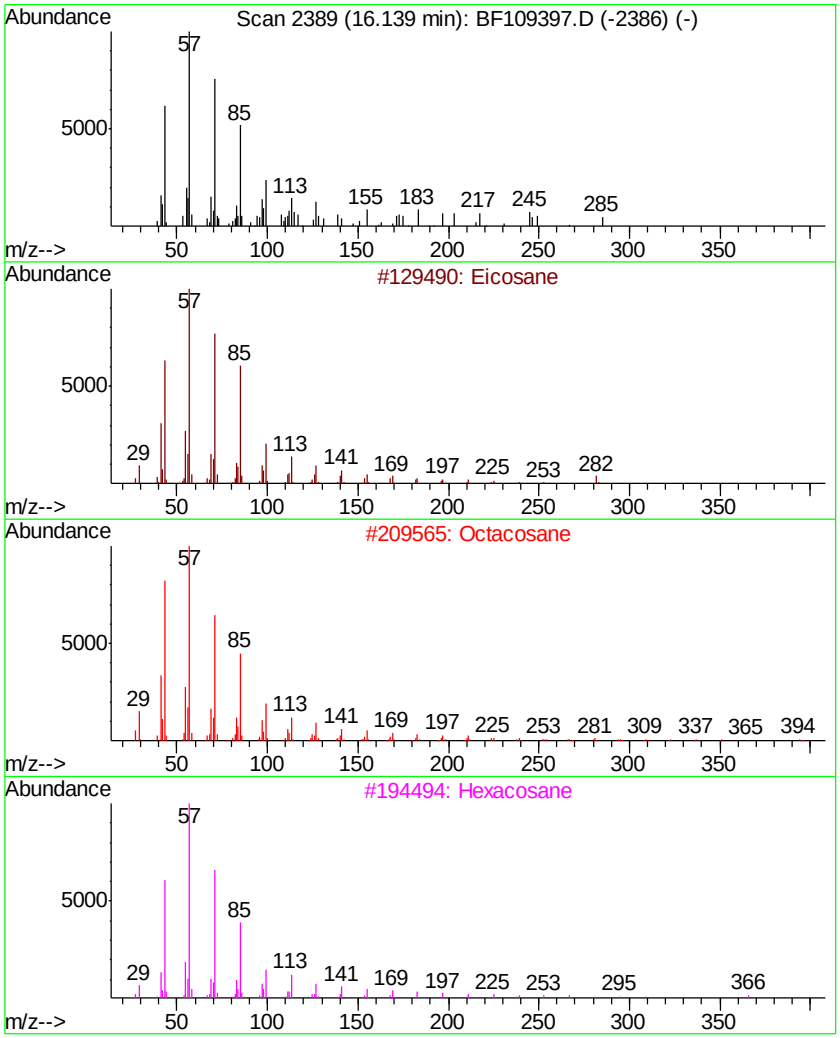
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

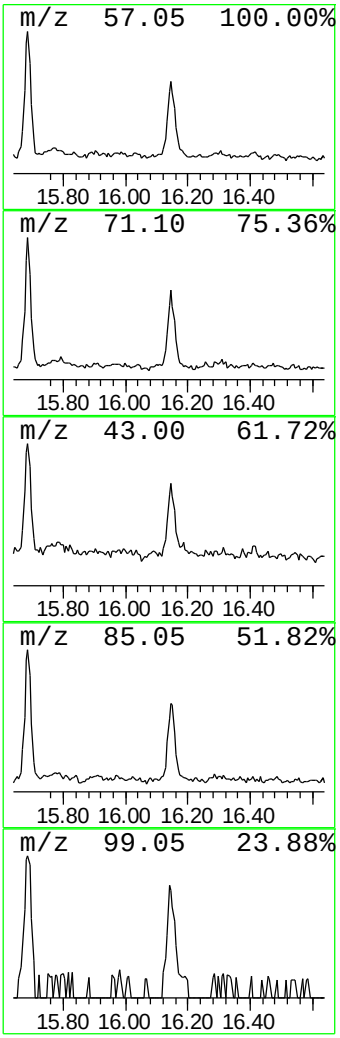
****

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.20 ng	76729	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octacosane	394	C28H58	000630-02-4	83
3	Hexacosane	366	C26H54	000630-01-3	81
4	Heneicosane	296	C21H44	000629-94-7	74
5	Pentacosane	352	C25H52	000629-99-2	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109397.D
Acq On : 27 Sep 2018 19:43
Operator : JU/SJ
Sample : J5077-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	2.1	ng	70519	1	6.70	675925	20.0
unknown6.47	6.47	54.9	ng	1855190	1	6.70	675925	20.0
Heptafluorobutyri...	13.71	3.6	ng	159451	5	13.84	891996	20.0
Squalene	14.69	8.0	ng	277747	6	15.24	698121	20.0
Heneicosane	14.93	2.5	ng	87191	6	15.24	698121	20.0
Hexacosane	15.69	2.6	ng	90210	6	15.24	698121	20.0
Eicosane	16.14	2.2	ng	76729	6	15.24	698121	20.0