LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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	3.581	248	254	262	rBV	158646	253558	6.68%	0.646%
2	4.846	465	469	485	rVB	266504	370285	9.75%	0.943%
3	5.275	538	542	556	rBV	3460271	3712545	97.77%	9.456%
4	5.504	576	581	586	rVB	111156	104668	2.76%	0.267%
5	6.257	706	709	714	rVB2	50733	45494	1.20%	0.116%
6	6.316	714	719	730	rBV	3639701	3797285	100.00%	9.672%
7	6.434	735	739	743	rVV	4076522	3638703	95.82%	9.268%
8	6.487	745	748	756	rVB2	106908	125688	3.31%	0.320%
9	6.663	774	778	785	rBV	1393915	1185130	31.21%	3.019%
10	6.716	785	787	794	rVB3	46264	58762	1.55%	0.150%
11	6.816	800	804	808	rBV	2899054	2543983	66.99%	6.479%
12	7.157	859	862	867	rBV2	35773	42636	1.12%	0.109%
13	7.228	870	874	879	rBV	2217860	2170531	57.16%	5.528%
14	7.710	952	956	961	rBV	69335	85023	2.24%	0.217%
15	7.945	992	996	999	rBV	1793324	1468973	38.68%	3.741%
16	8.875	1151	1154	1161	rBV	66802	76024	2.00%	0.194%
17	9.022	1174	1179	1182	rBV	3517396	2882291	75.90%	7.341%
18	9.416	1243	1246	1250	rVB	446180	355522	9.36%	0.906%
19	9.633	1280	1283	1286	rBV	39656	42446	1.12%	0.108%
20	9.692	1289	1293	1297	rVV	1460420	1311006	34.52%	3.339%
21	10.128	1365	1367	1370	rBV	57508	45244	1.19%	0.115%
22	10.239	1383	1386	1392	rVB	44474	52463	1.38%	0.134%
23	10.363	1401	1407	1410	rBV	1601260	1650197	43.46%	4.203%
24	10.480	1422	1427	1436	rBV	1418902	1430521	37.67%	3.644%
25	10.563	1436	1441	1444	rVV	1843624	1980677	52.16%	5.045%
26	10.604	1445	1448	1456	rVB	102473	174648	4.60%	0.445%
27	11.075	1526	1528	1534	rVB2	41307	41473	1.09%	0.106%
28	11.175	1541	1545	1547	rBV	1278179	1087588	28.64%	2.770%
29	11.198	1547	1549	1552	rVV	416384	321220	8.46%	0.818%
30	11.251	1552	1558	1561	rVB	98661	107506	2.83%	0.274%
31	11.416	1581	1586	1590	rBV2	34347	48346	1.27%	0.123%
32	11.675	1627	1630	1632	rBV	54559	44223	1.16%	0.113%
33	11.704	1632	1635	1639	rVB	68607	61839	1.63%	0.158%
34	11.751	1639	1643	1645	rBV2	32922	39048	1.03%	0.099%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.786	1646	1649	1651	rBV	104148	91157	2.40%	0.232%
36	12.222	1720	1723	1726	rBV2	46566	53985	1.42%	0.137%
37	12.386	1747	1751	1755	rBV	750729	638586	16.82%	1.626%
38	12.610	1784	1789	1792	rBV	581142	585894	15.43%	1.492%
39	12.663	1796	1798	1802	rVB2	53283	55131	1.45%	0.140%
40	12.757	1810	1814	1822	rVB	2180590	1942964	51.17%	4.949%
41	12.833	1823	1827	1831	rBV3	38472	64641	1.70%	0.165%
42	12.939	1843	1845	1849	rVB	129786	113746	3.00%	0.290%
43	13.010	1853	1857	1859	rVV	109152	103695	2.73%	0.264%
44	13.045	1859	1863	1867	rVV2	61544	79795	2.10%	0.203%
45	13.163	1881	1883	1886	rBV2	34087	38954	1.03%	0.099%
46	13.363	1915	1917	1923	rVB7	30835	44934	1.18%	0.114%
47	13.451	1930	1932	1936	rVB3	36647	41931	1.10%	0.107%
48	13.557	1948	1950	1953	rBV	58325	58362	1.54%	0.149%
49	13.657	1964	1967	1971	rVB2	156532	161127	4.24%	0.410%
50	13.810	1987	1993	1995	rBV2	1222458	1434750	37.78%	3.654%
51	13.833	1995	1997	2000	rVB	311755	252768	6.66%	0.644%
52	13.910	2008	2010	2013	rVB	68849	58528	1.54%	0.149%
53	14.192	2056	2058	2061	rVB	55402	49437	1.30%	0.126%
54	14.286	2071	2074	2077	rBV2	75693	82239	2.17%	0.209%
55	14.815	2160	2164	2167	rBV	247376	355715	9.37%	0.906%
56	14.886	2173	2176	2178	rVB	65649	63277	1.67%	0.161%
57	15.092	2208	2211	2217	rVV	131274	154694	4.07%	0.394%
58	15.151	2218	2221	2226	rVV	218203	245697	6.47%	0.626%
59	15.210	2226	2231	2243	rVB	740546	1002206	26.39%	2.553%
60	16.551	2455	2459	2464	rVB3	77801	132296	3.48%	0.337%

Sum of corrected areas: 39262055

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Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
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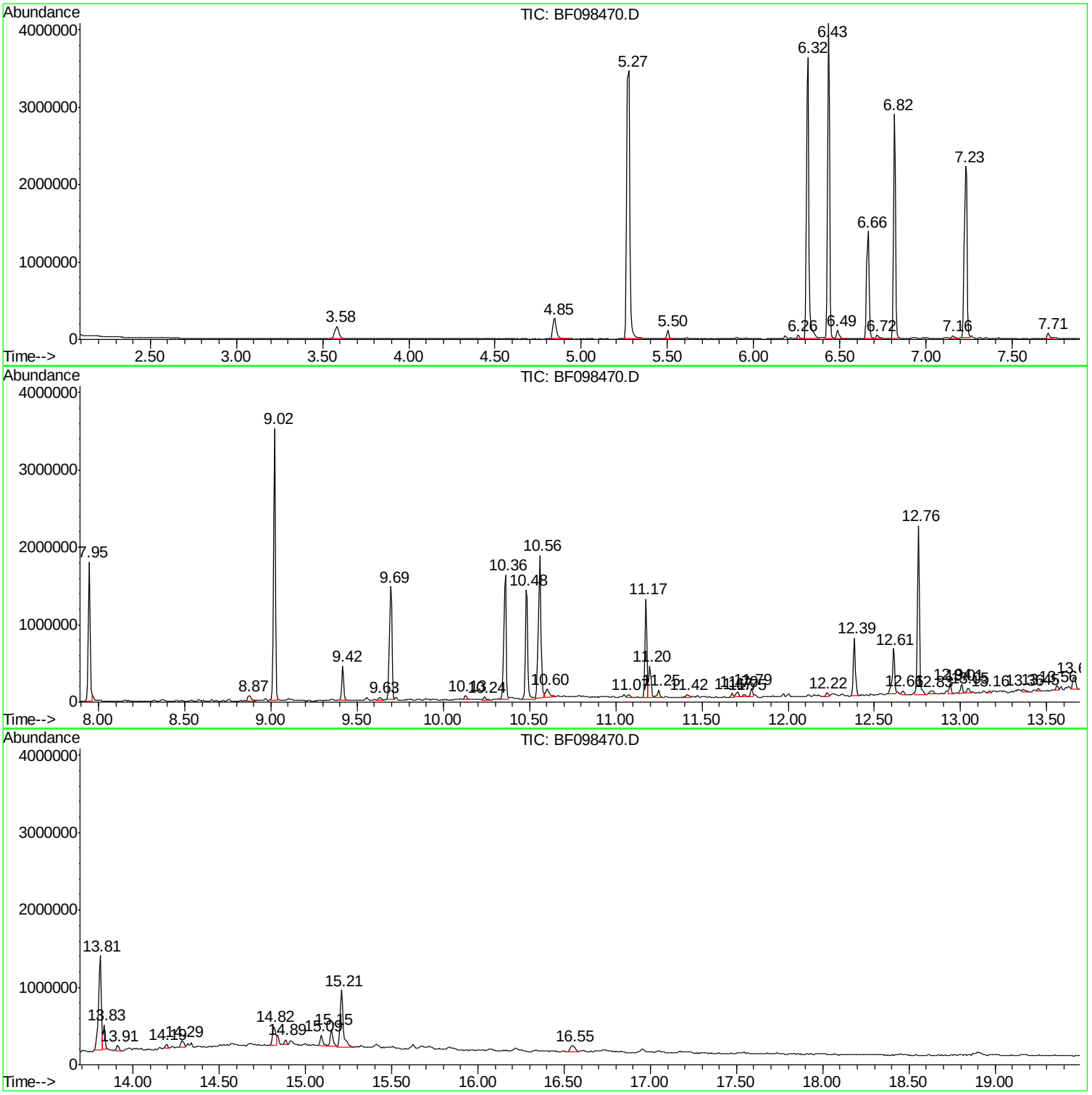
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

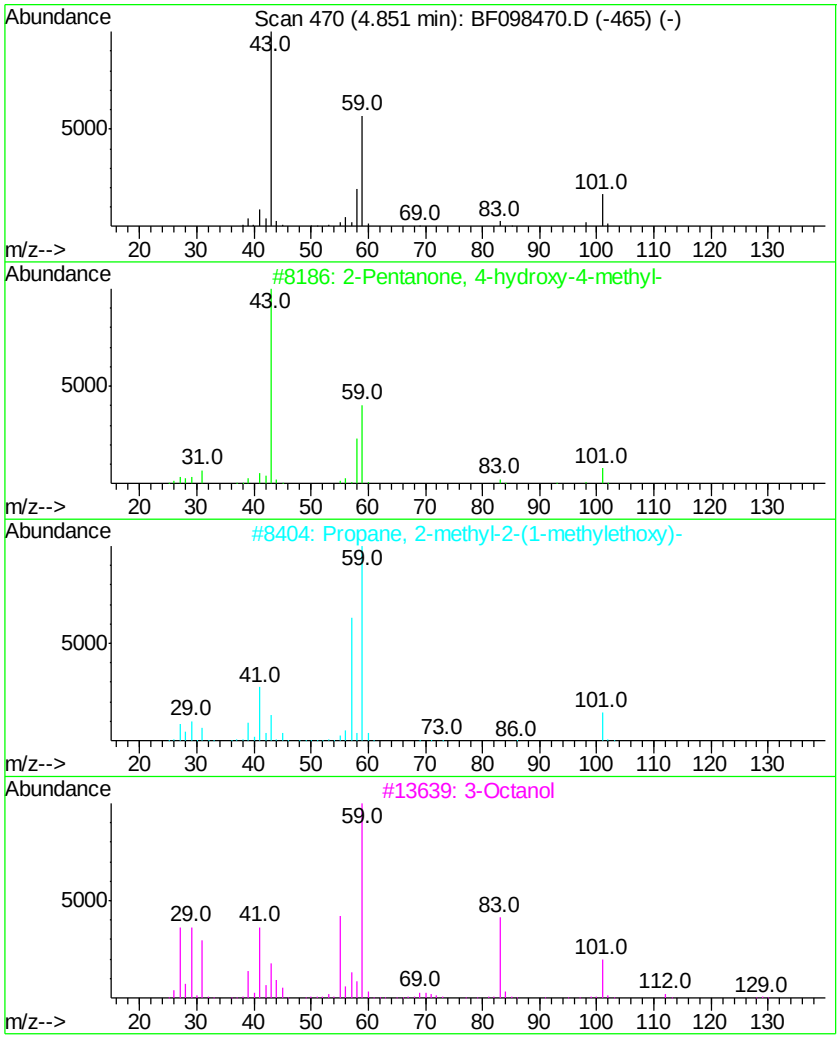
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

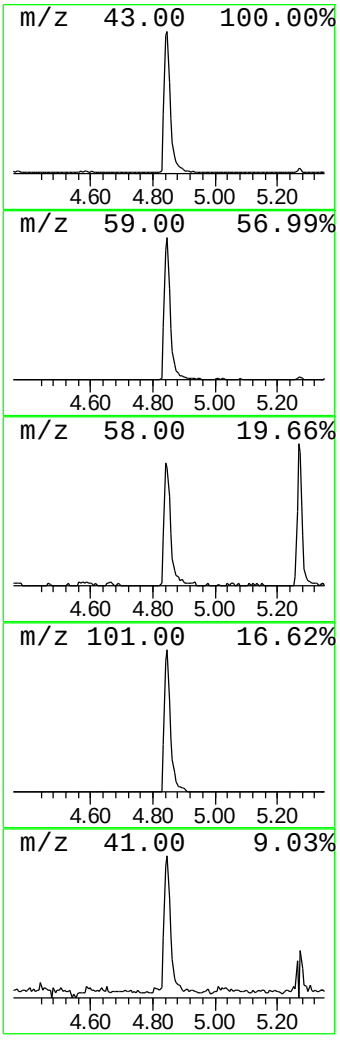
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	6.25 ng	370285	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

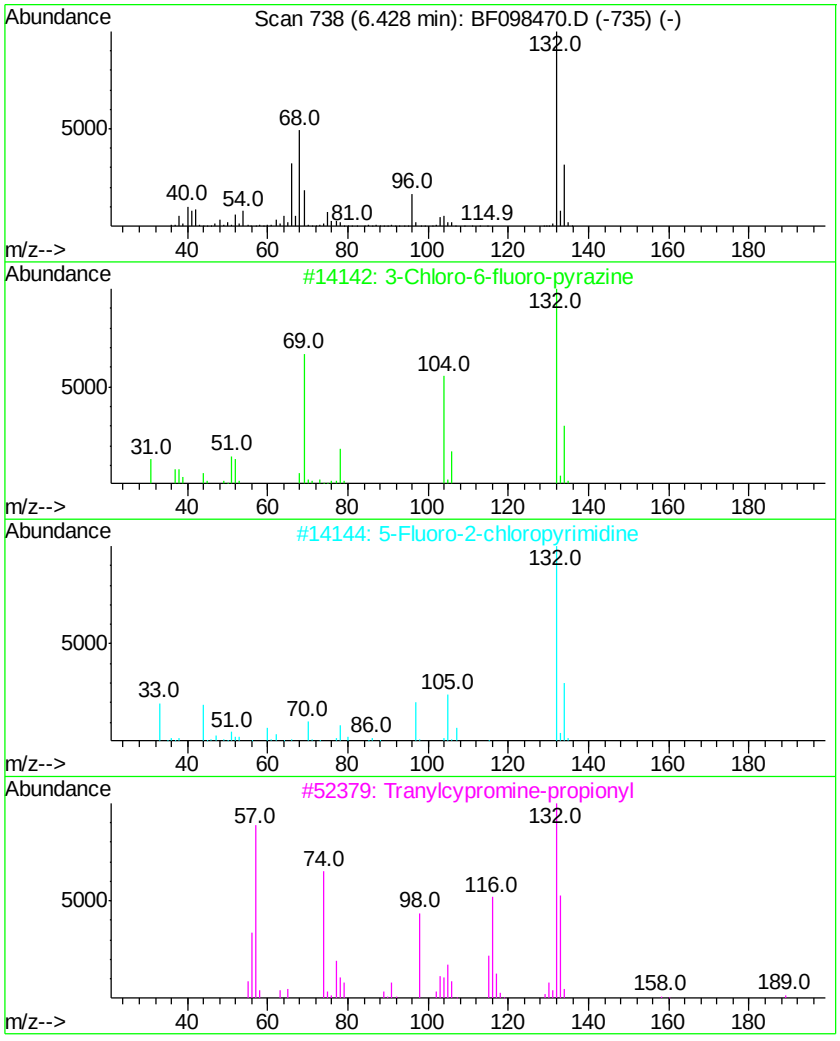
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

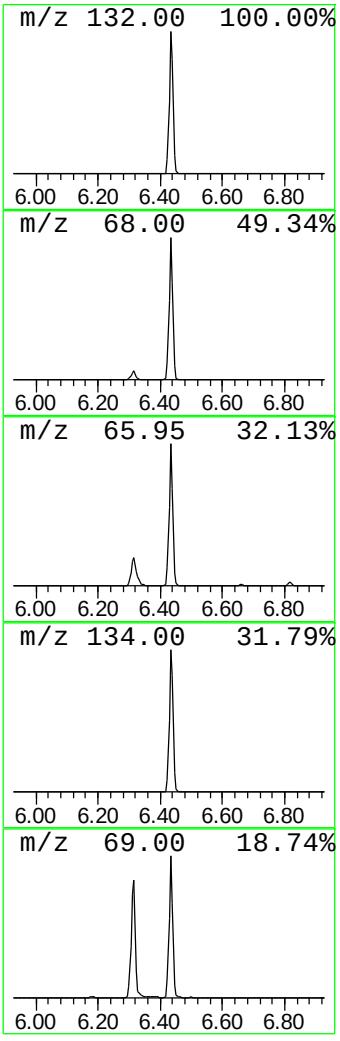
****

Peak Number 3 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	61.41 ng	3638700	1,4-Dichlorobenzene-d4	6.66

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

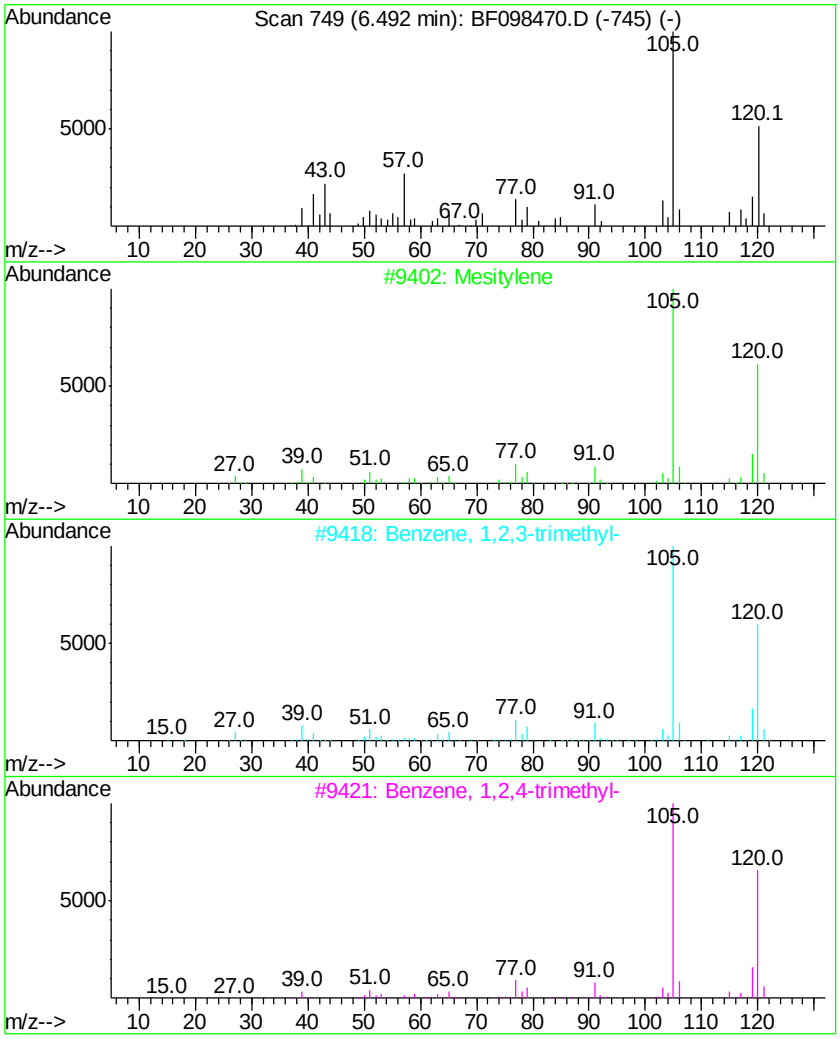
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

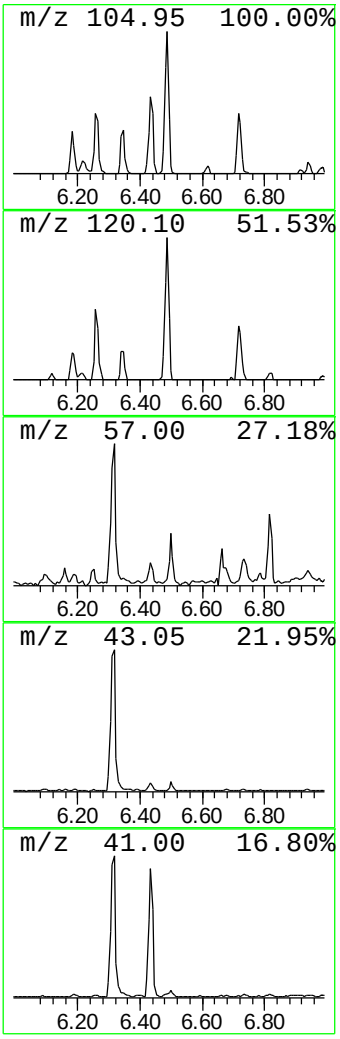
****

Peak Number 4 Mesitylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	2.12 ng	125688	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

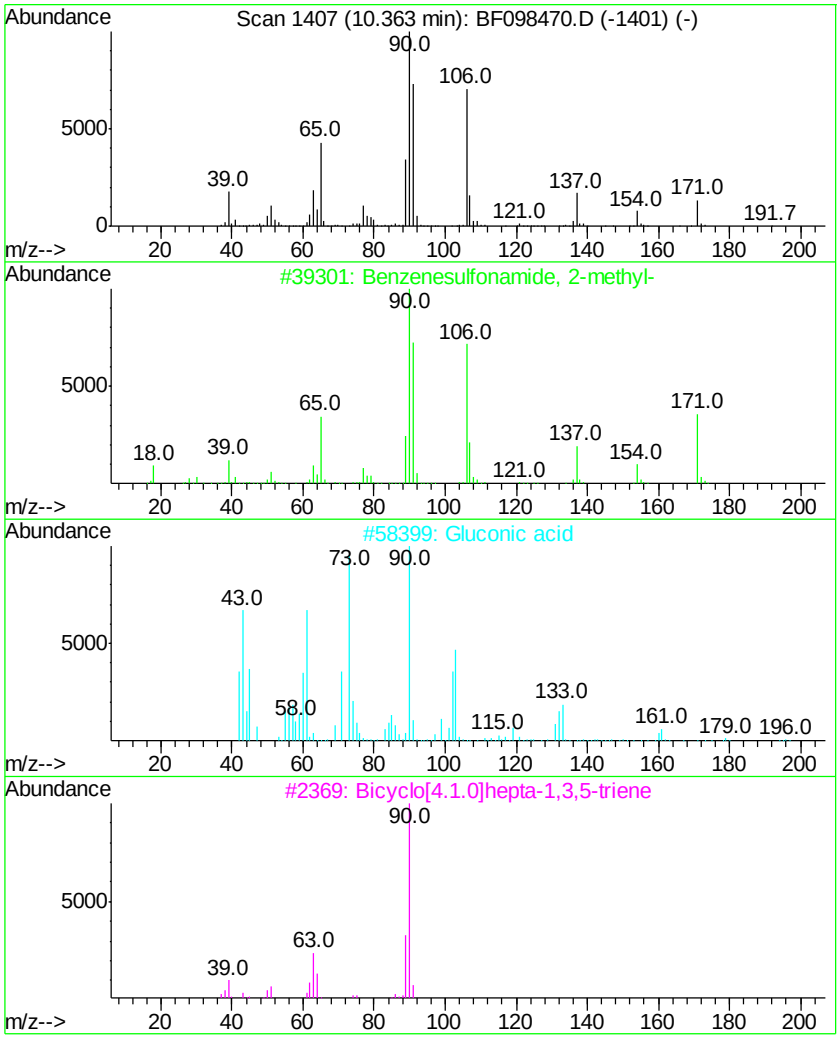
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

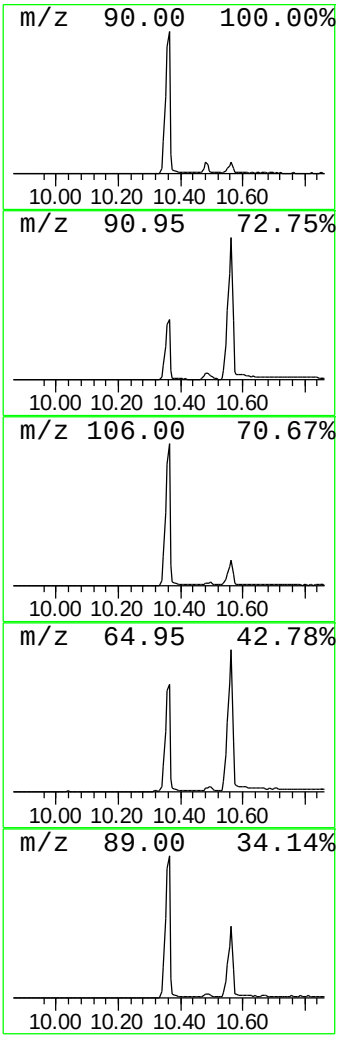
****

Peak Number 6 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	25.17 ng	1650200	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	97
2	Gluconic acid	196	C6H12O7	000526-95-4	43
3	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
4	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	38
5	Thiourea, methyl-	90	C2H6N2S	000598-52-7	25





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

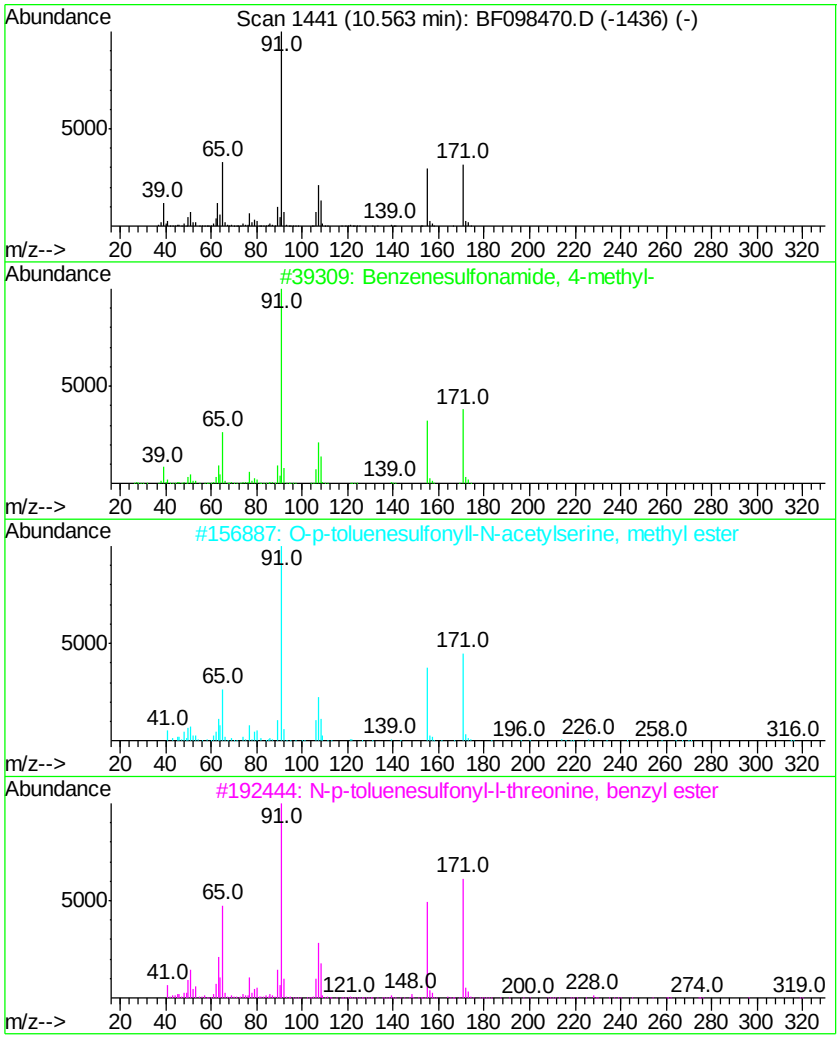
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

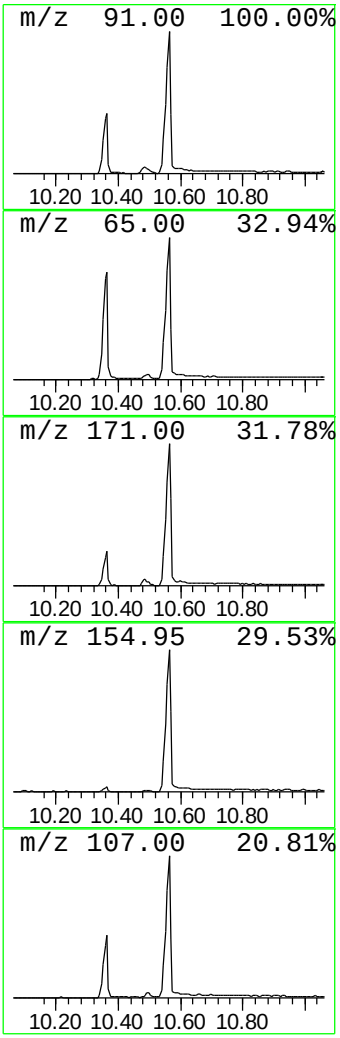
****

Peak Number 7 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	36.42 ng	1980680	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	83
3	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	83
4	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	80
5	Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	43





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

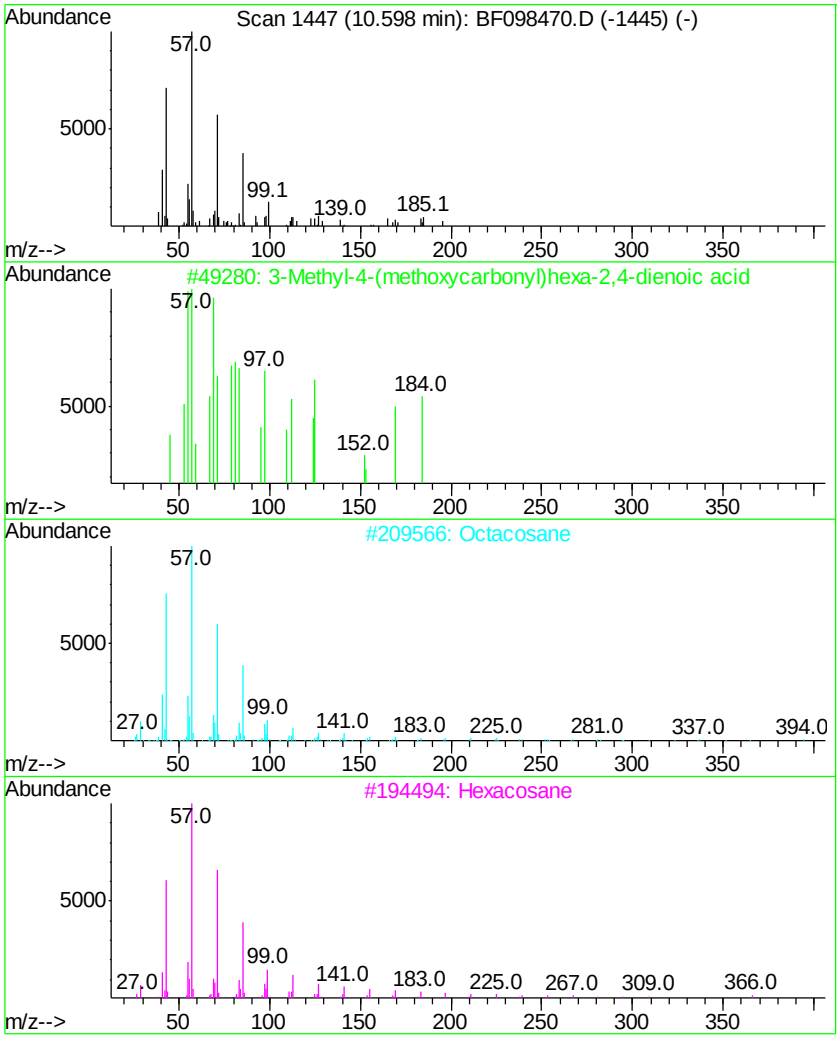
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

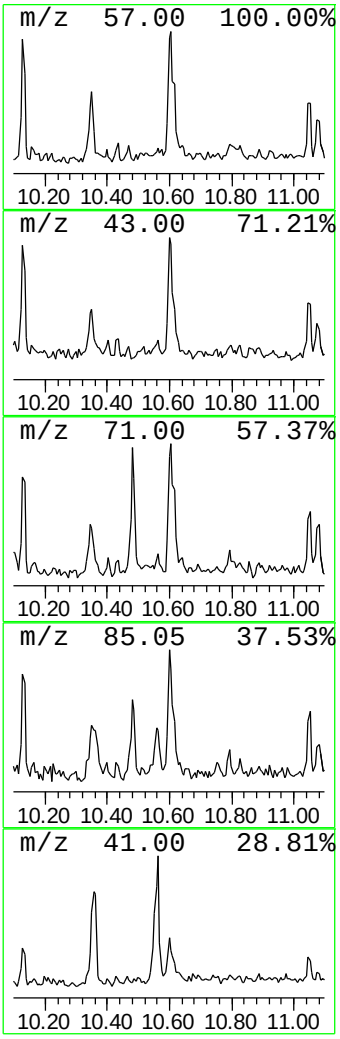
****

Peak Number 8 3-Methyl-4-(methoxycarbonyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	3.21 ng	174648	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	87
2	Octacosane	394	C28H58	000630-02-4	74
3	Hexacosane	366	C26H54	000630-01-3	72
4	Heptacosane	380	C27H56	000593-49-7	68
5	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	64





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Data File : BF098470.D
Acq On : 13 Sep 2017 00:29
Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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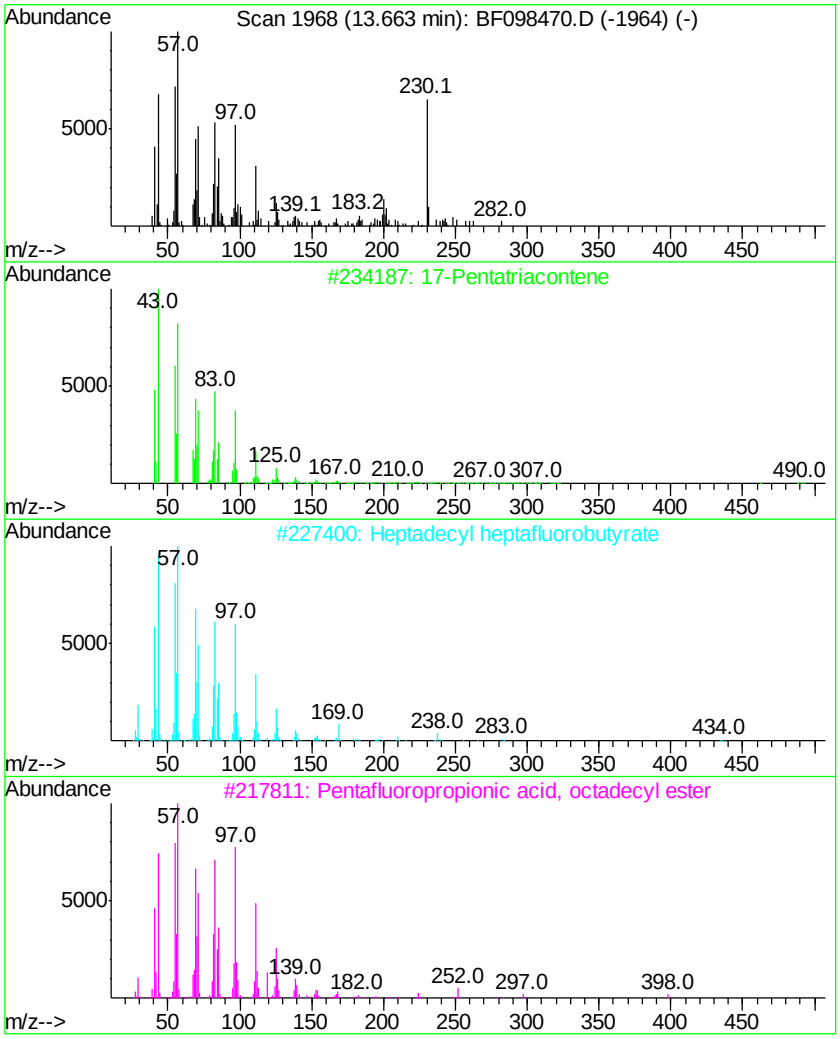
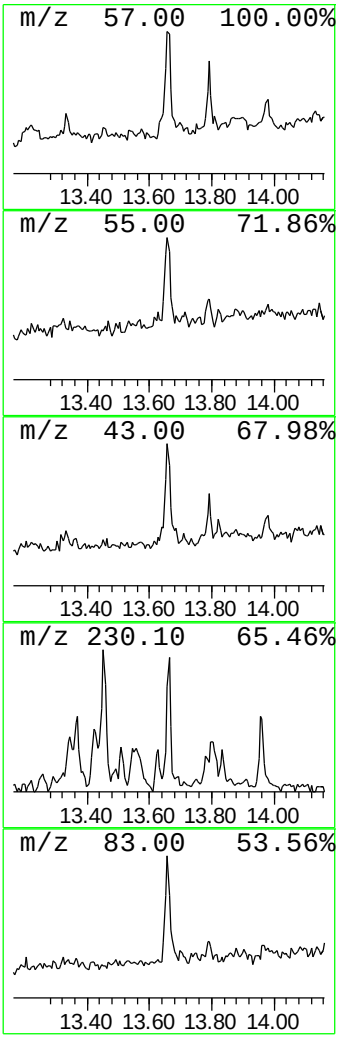
Peak Number 9 17-Pentatriacontene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.25 ng	161127	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	83
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	83
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091217\
Data File : BF098470.D
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Operator : SJ/JU
Sample : I5140-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-0-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.85	6.3	ng	370285	1	6.66	1185130	20.0
unknown6.43	6.43	61.4	ng	3638700	1	6.66	1185130	20.0
Mesitylene	6.49	2.1	ng	125688	1	6.66	1185130	20.0
Benzenesulfonamid...	10.36	25.2	ng	1650200	3	9.69	1311010	20.0
Benzenesulfonamid...	10.56	36.4	ng	1980680	4	11.17	1087590	20.0
3-Methyl-4-(metho...	10.60	3.2	ng	174648	4	11.17	1087590	20.0
17-Pentatriacontene	13.66	2.3	ng	161127	5	13.81	1434750	20.0