LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117967.D
Acq On : 23 Nov 2019 20:04
Operator : JU
Sample : K5927-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

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-BF111319.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	2.163	8	13	44	rVB	558155	1004394	36.72%	3.207%
2	5.110	509	514	523	rVB	340798	396653	14.50%	1.267%
3	5.510	578	582	586	rBV	2126573	2041686	74.65%	6.520%
4	6.522	749	754	757	rBV	2040062	1795951	65.67%	5.735%
5	6.669	775	779	782	rBV	2271415	1895456	69.31%	6.053%
6	6.904	815	819	822	rBV	756720	661305	24.18%	2.112%
7	7.057	841	845	849	rBV	1768226	1456621	53.26%	4.651%
8	7.463	910	914	917	rBV	1339142	1105261	40.41%	3.529%
9	8.192	1034	1038	1041	rBV	903978	868921	31.77%	2.775%
10	9.269	1217	1221	1224	rBV	2692039	2246115	82.13%	7.172%
11	9.663	1284	1288	1295	rVB	363358	317700	11.62%	1.014%
12	9.951	1333	1337	1340	rBV	1222357	1017652	37.21%	3.250%
13	9.986	1340	1343	1346	rVB	103425	95432	3.49%	0.305%
14	10.157	1367	1372	1376	rBV	75418	71958	2.63%	0.230%
15	10.498	1427	1430	1436	rBV	98142	94124	3.44%	0.301%
16	10.739	1467	1471	1485	rBV	1645105	1621226	59.28%	5.177%
17	11.051	1518	1524	1527	rBV3	21797	29087	1.06%	0.093%
18	11.304	1561	1567	1569	rBV3	20673	29323	1.07%	0.094%
19	11.339	1571	1573	1579	rVB	58788	46775	1.71%	0.149%
20	11.445	1587	1591	1593	rBV	1307907	1134667	41.49%	3.623%
21	11.468	1593	1595	1598	rVV	1086398	813139	29.73%	2.597%
22	11.521	1598	1604	1607	rVV	255928	283338	10.36%	0.905%
23	11.551	1607	1609	1613	rVB	33352	32823	1.20%	0.105%
24	11.674	1624	1630	1638	rBV2	125112	150689	5.51%	0.481%
25	11.945	1671	1676	1677	rBV	94003	78630	2.88%	0.251%
26	11.968	1677	1680	1686	rVB2	302698	357851	13.08%	1.143%
27	12.021	1686	1689	1692	rVB	66253	55734	2.04%	0.178%
28	12.063	1692	1696	1698	rBV	154341	162261	5.93%	0.518%
29	12.245	1724	1727	1729	rBV	63532	48658	1.78%	0.155%
30	12.498	1764	1770	1773	rBV2	51519	58821	2.15%	0.188%
31	12.539	1773	1777	1779	rVV2	34184	42221	1.54%	0.135%
32	12.580	1782	1784	1790	rVB2	26244	36293	1.33%	0.116%
33	12.663	1794	1798	1801	rBV	1054599	862138	31.52%	2.753%
34	12.751	1811	1813	1817	rBV2	80362	79823	2.92%	0.255%

LSC Area Percent Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

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
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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.892	1831	1837	1840	rBV	917623	923653	33.77%	2.949%
36	12.939	1843	1845	1850	rVB2	51637	54830	2.00%	0.175%
37	13.033	1857	1861	1868	rVB	3007341	2734946	100.00%	8.733%
38	13.104	1868	1873	1877	rBV2	47652	84305	3.08%	0.269%
39	13.198	1882	1889	1890	rBV4	41979	59104	2.16%	0.189%
40	13.221	1890	1893	1896	rVB2	148927	133888	4.90%	0.428%
41	13.286	1901	1904	1907	rBV	130451	107231	3.92%	0.342%
42	13.321	1907	1910	1913	rVV2	81297	84663	3.10%	0.270%
43	13.415	1923	1926	1929	rBV	42980	38652	1.41%	0.123%
44	13.451	1929	1932	1935	rBV2	46356	50783	1.86%	0.162%
45	13.704	1972	1975	1978	rBV2	24439	38559	1.41%	0.123%
46	13.845	1993	1999	2001	rBV2	48698	58715	2.15%	0.187%
47	13.868	2001	2003	2005	rVV	75981	63161	2.31%	0.202%
48	13.904	2005	2009	2011	rVV2	48999	79108	2.89%	0.253%
49	13.933	2011	2014	2022	rVB3	146111	217045	7.94%	0.693%
50	14.092	2036	2041	2044	rBV2	1375588	1551769	56.74%	4.955%
51	14.115	2044	2045	2051	rVB	404891	326031	11.92%	1.041%
52	14.198	2053	2059	2062	rBV	80467	71846	2.63%	0.229%
53	14.251	2065	2068	2071	rBV4	30295	29261	1.07%	0.093%
54	14.280	2071	2073	2076	rVB	33475	28766	1.05%	0.092%
55	14.315	2076	2079	2083	rVB2	39882	53074	1.94%	0.169%
56	14.480	2103	2107	2110	rBV	83141	86773	3.17%	0.277%
57	14.515	2110	2113	2116	rVB	44614	41659	1.52%	0.133%
58	14.562	2116	2121	2126	rBV4	60152	125417	4.59%	0.400%
59	14.627	2130	2132	2136	rVV3	56780	53750	1.97%	0.172%
60	14.680	2136	2141	2146	rVB4	31016	52310	1.91%	0.167%
61	14.798	2156	2161	2163	rBV5	26081	37990	1.39%	0.121%
62	14.874	2171	2174	2177	rBV2	52435	49617	1.81%	0.158%
63	14.951	2184	2187	2191	rBV	42595	47340	1.73%	0.151%
64	15.151	2215	2221	2224	rBV	266771	423757	15.49%	1.353%
65	15.227	2230	2234	2237	rBV2	56279	65632	2.40%	0.210%
66	15.262	2237	2240	2244	rVB	58232	65454	2.39%	0.209%
67	15.462	2269	2274	2280	rVB	161011	213352	7.80%	0.681%
68	15.527	2280	2285	2291	rBV	258275	307856	11.26%	0.983%
69	15.598	2291	2297	2300	rBV	724854	949081	34.70%	3.031%
70	15.621	2300	2301	2308	rVB2	122898	138563	5.07%	0.442%
71	16.080	2375	2379	2384	rVB3	43455	65117	2.38%	0.208%

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Instrument : BNA_F
ClientSampleId : B-8

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.609	2464	2469	2475	rVB3	37034	64171	2.35%	0.205%
73	17.109	2548	2554	2562	rVB2	112237	228197	8.34%	0.729%
74	17.221	2570	2573	2579	rVB5	22154	45842	1.68%	0.146%
75	17.297	2581	2586	2592	rVV	31871	75305	2.75%	0.240%
76	17.356	2592	2596	2602	rVV3	35113	81613	2.98%	0.261%
77	17.403	2602	2604	2614	rVB10	22362	45760	1.67%	0.146%
78	17.568	2625	2632	2645	rBV	76136	181740	6.65%	0.580%
79	17.809	2668	2673	2680	rVB2	28129	57396	2.10%	0.183%
80	17.962	2695	2699	2704	rVB7	16226	30707	1.12%	0.098%

Sum of corrected areas: 31316515

LSC Report - Integrated Chromatogram

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Data File : BF117967.D
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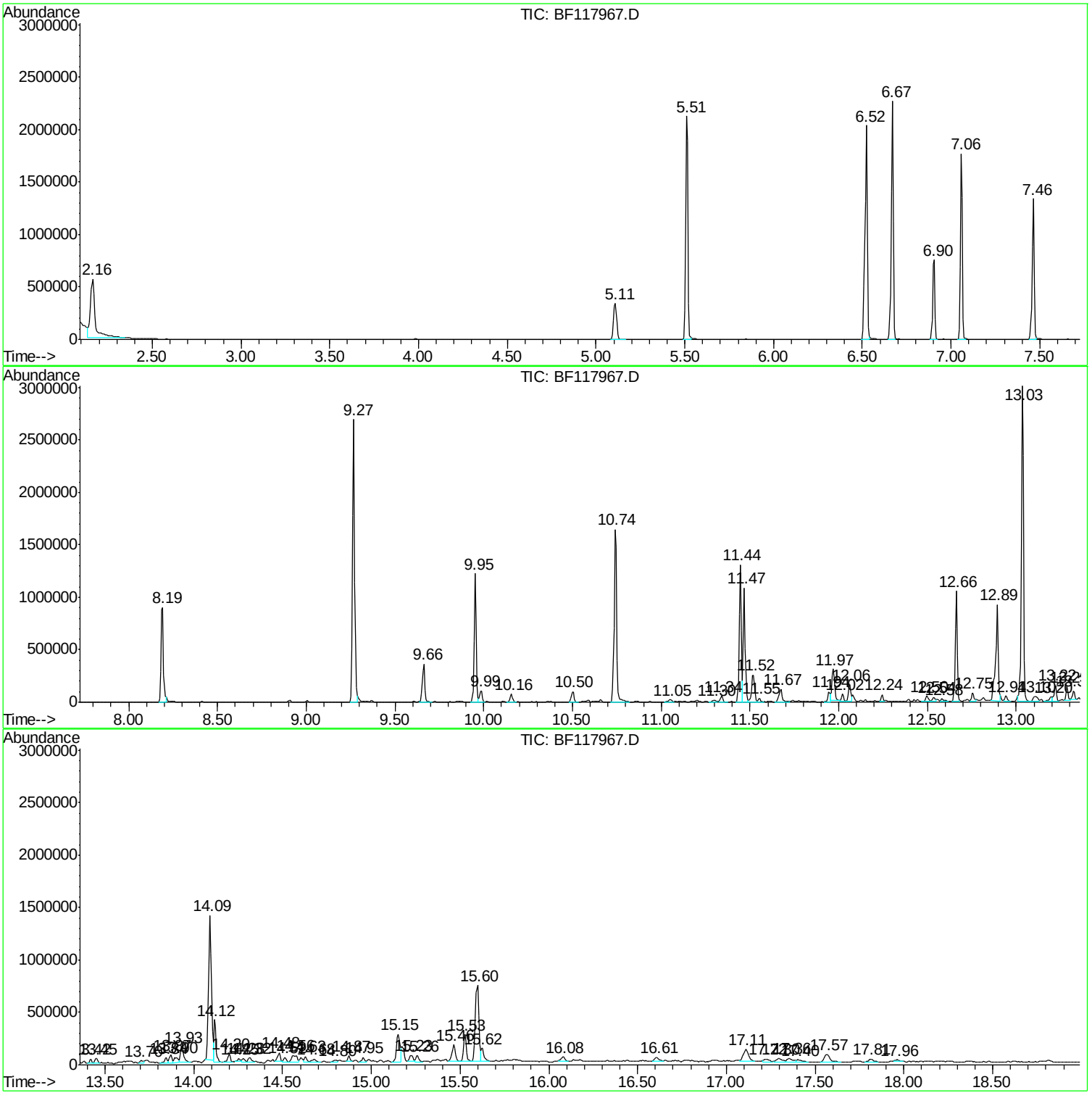
Sample : K5927-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112319\
Data File : BF117967.D
Acq On : 23 Nov 2019 20:04
Operator : JU
Sample : K5927-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

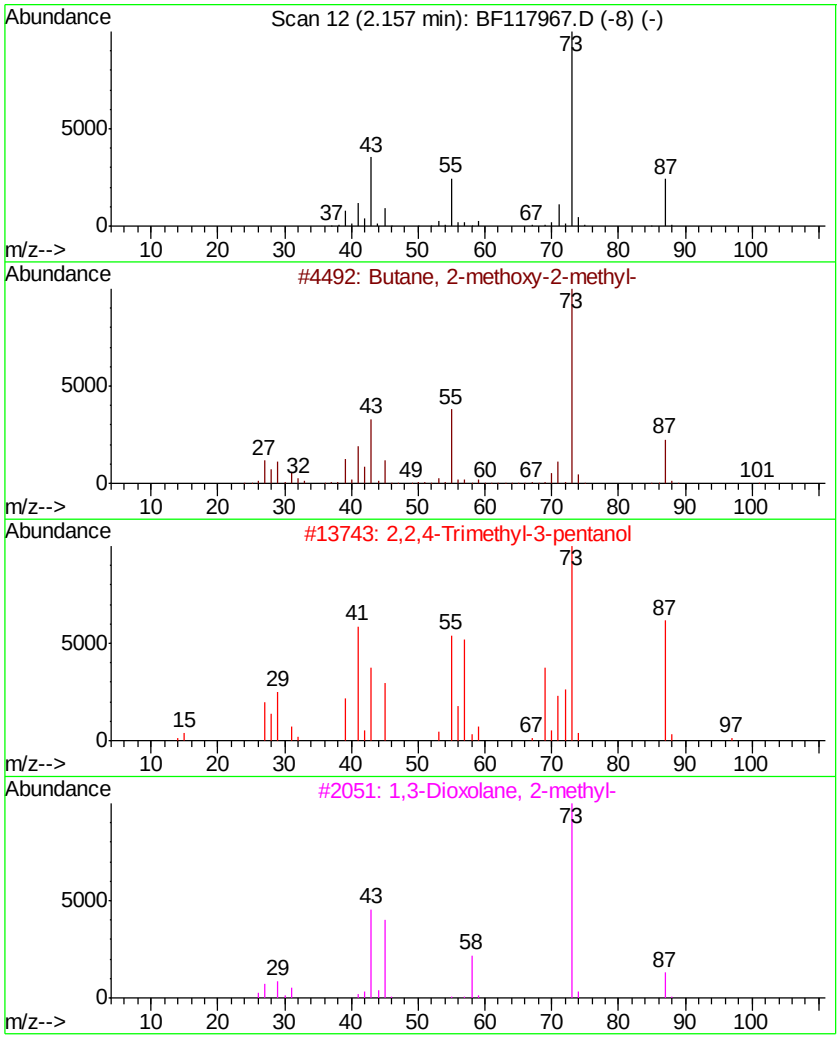
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

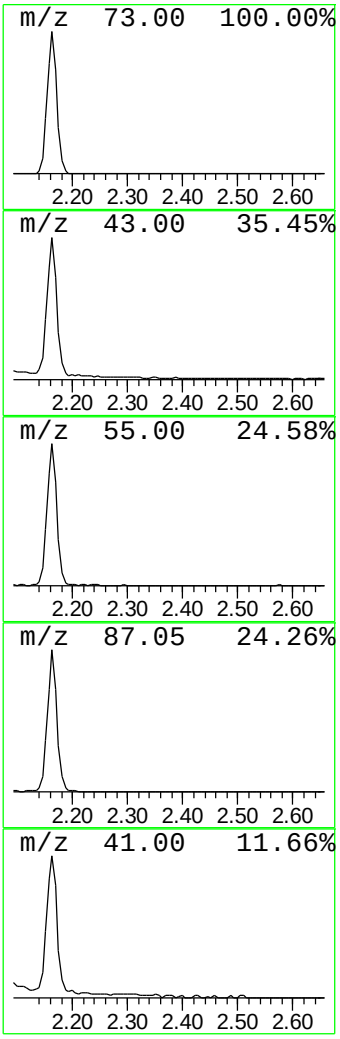
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	30.38 ng	1004390	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Library Search Compound Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

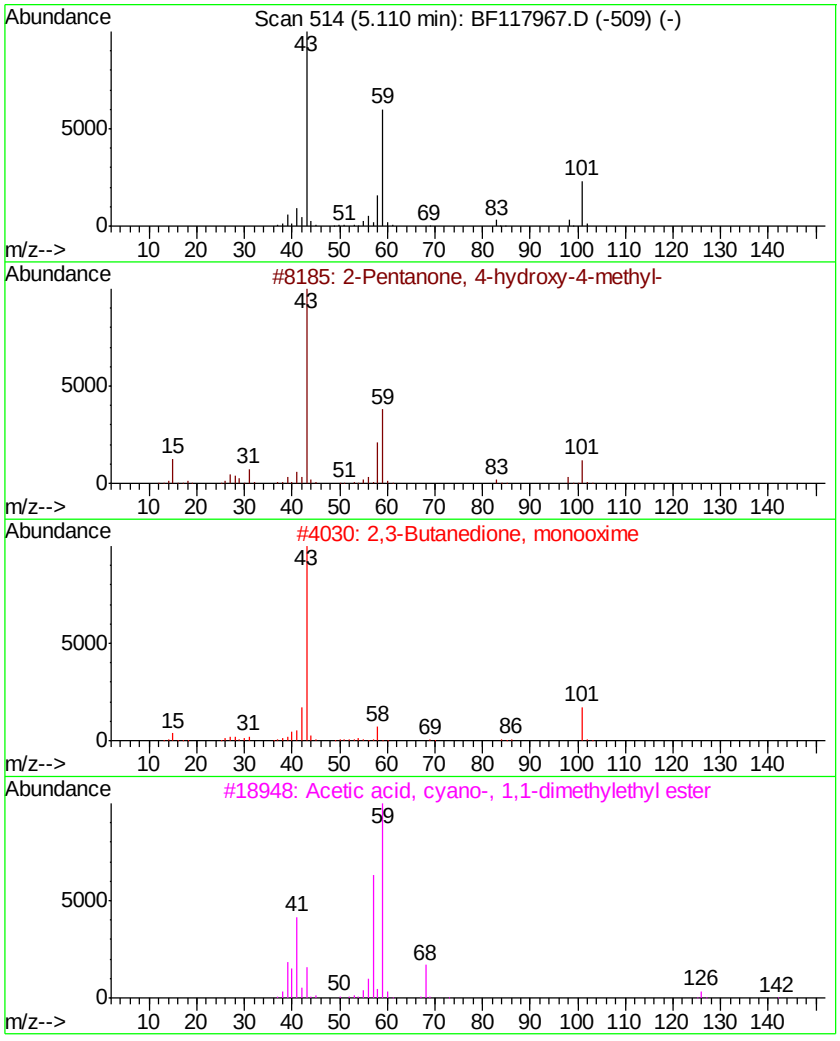
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

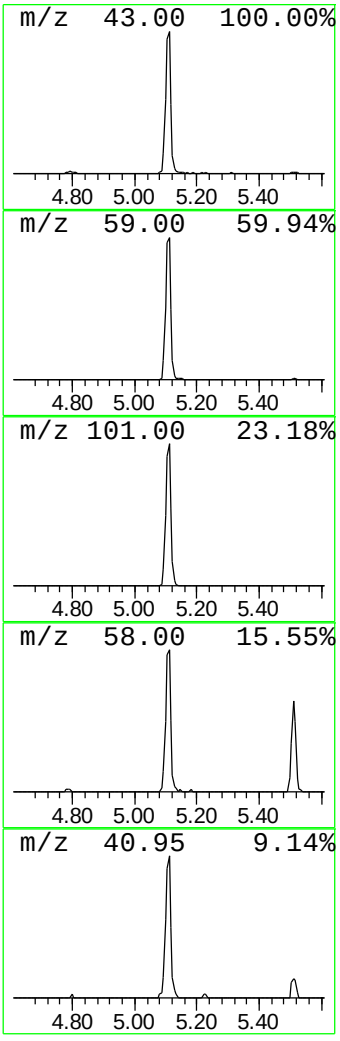
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.00 ng	396653	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
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Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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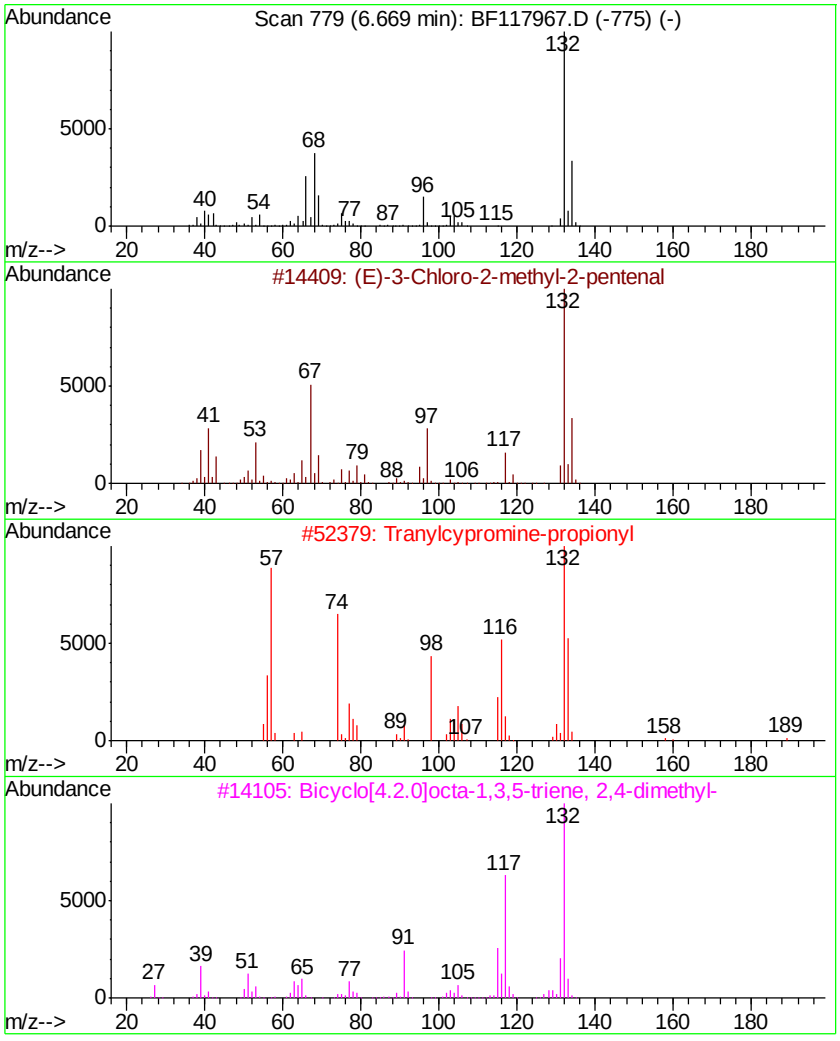
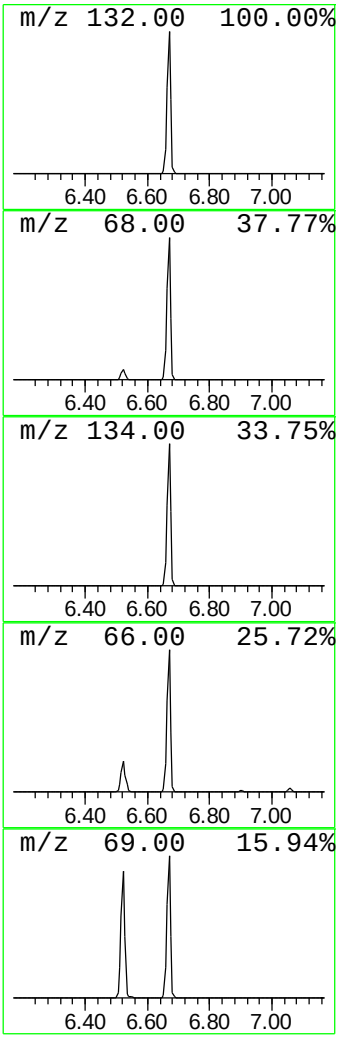
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	57.32 ng	1895460	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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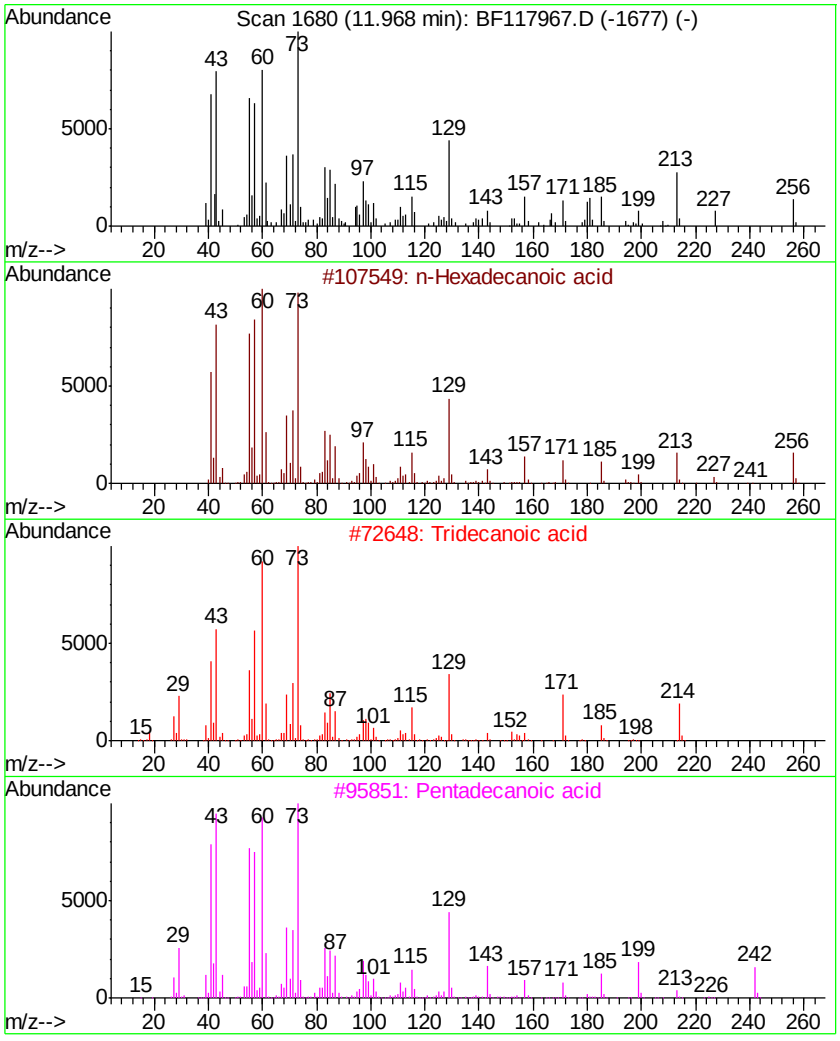
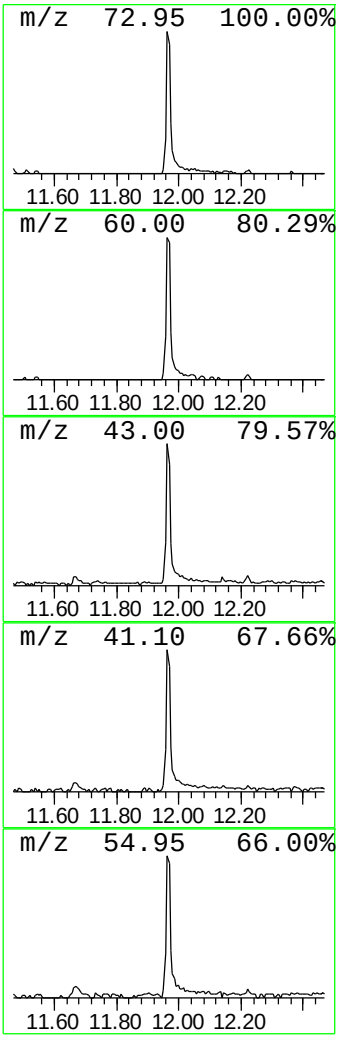
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	6.31 ng	357851	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

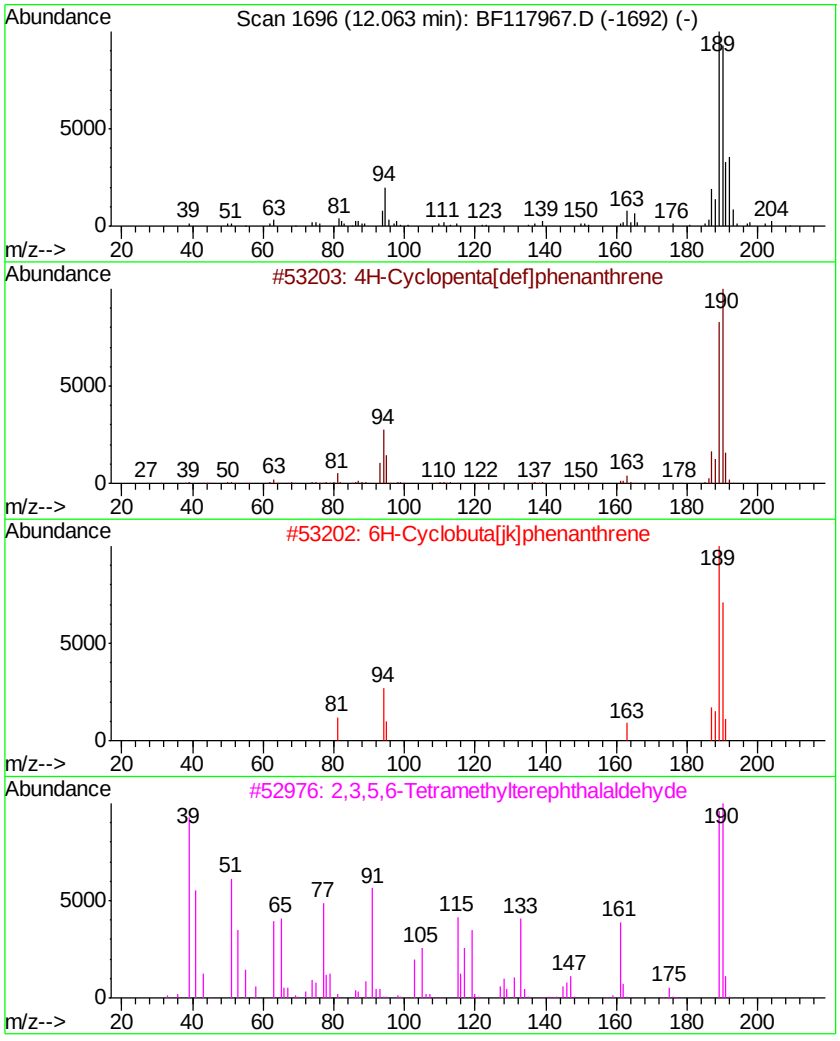
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

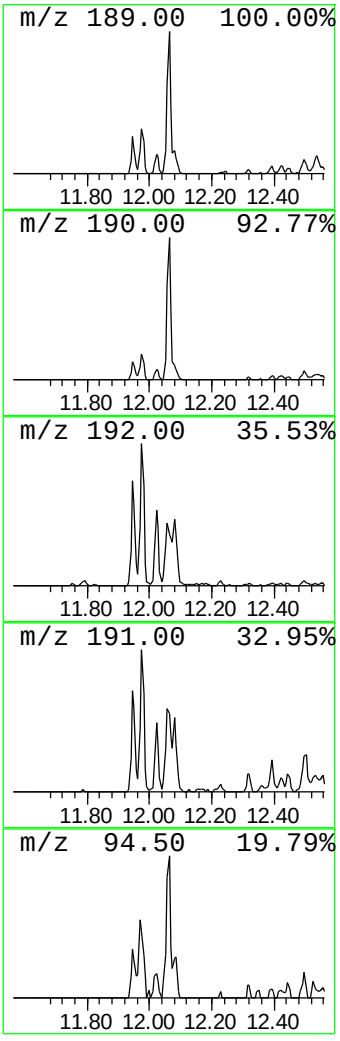
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	2.86 ng	162261	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
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Sample : K5927-10
Misc :
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Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

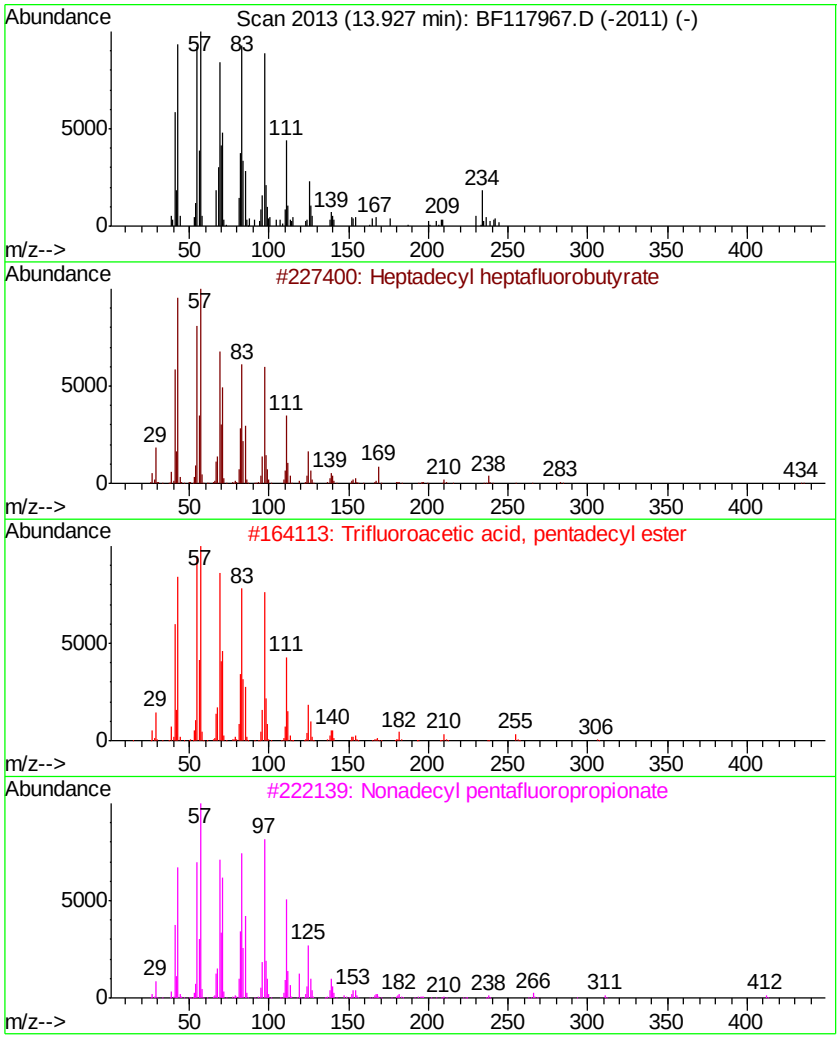
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

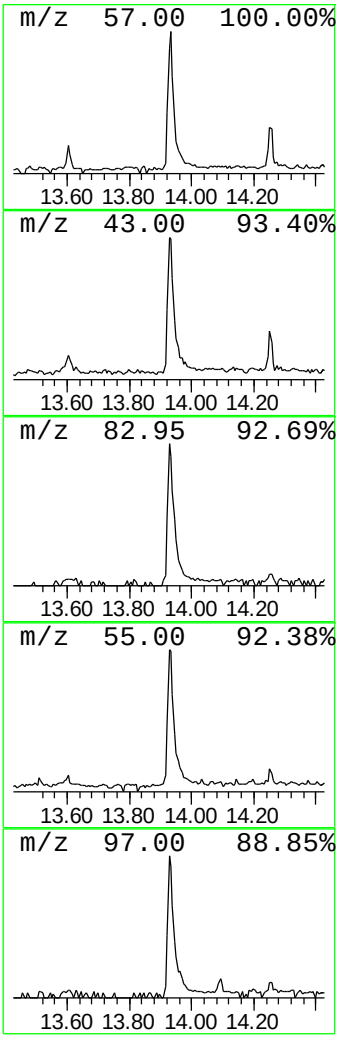
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.80 ng	217045	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112319\
Data File : BF117967.D
Acq On : 23 Nov 2019 20:04
Operator : JU
Sample : K5927-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.16	30.4	ng	1004390	1	6.90	661305	20.0
2-Pentanone, 4-hy...	5.11	12.0	ng	396653	1	6.90	661305	20.0
unknown6.67	6.67	57.3	ng	1895460	1	6.90	661305	20.0
n-Hexadecanoic acid	11.97	6.3	ng	357851	4	11.44	1134670	20.0
4H-Cyclopenta[def...	12.06	2.9	ng	162261	4	11.44	1134670	20.0
Heptadecyl heptaf...	13.93	2.8	ng	217045	5	14.09	1551770	20.0