LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

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-BF022218.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	4.487	403	408	419	rBV2	41385	98301	3.15%	0.367%
2	4.581	419	424	441	rVV	645598	985977	31.59%	3.678%
3	5.075	504	508	529	rBV	665261	931822	29.85%	3.476%
4	5.510	578	582	611	rBV	154065	627827	20.11%	2.342%
5	5.751	620	623	631	rVB	42319	48924	1.57%	0.183%
6	6.269	707	711	717	rBV4	24263	45433	1.46%	0.169%
7	6.504	748	751	769	rBV	1758955	3121452	100.00%	11.644%
8	6.633	769	773	786	rVB	1641641	2146262	68.76%	8.006%
9	6.857	808	811	820	rBV	623812	847166	27.14%	3.160%
10	7.010	833	837	852	rBV	2149434	2505890	80.28%	9.348%
11	7.175	862	865	869	rVB3	25935	33534	1.07%	0.125%
12	7.428	904	908	931	rBV	1607461	2296091	73.56%	8.565%
13	7.580	931	934	938	rVB	34167	37201	1.19%	0.139%
14	7.739	954	961	963	rBV2	57409	57858	1.85%	0.216%
15	8.033	1008	1011	1016	rBV	291474	257597	8.25%	0.961%
16	8.139	1026	1029	1049	rBV	880088	1172982	37.58%	4.376%
17	9.216	1208	1212	1220	rBV	2964157	3116281	99.83%	11.625%
18	9.280	1220	1223	1228	rVB	72152	80294	2.57%	0.300%
19	9.610	1273	1279	1285	rBV	243898	290174	9.30%	1.082%
20	9.810	1309	1313	1317	rBV	137575	109418	3.51%	0.408%
21	9.898	1324	1328	1333	rBV2	1113004	1108586	35.52%	4.135%
22	10.127	1364	1367	1372	rVB3	30556	41835	1.34%	0.156%
23	10.310	1395	1398	1401	rVB	162310	130803	4.19%	0.488%
24	10.527	1430	1435	1438	rBV	49915	63581	2.04%	0.237%
25	10.704	1461	1465	1470	rBV3	95584	134117	4.30%	0.500%
26	10.780	1475	1478	1487	rVB	134894	179809	5.76%	0.671%
27	11.233	1551	1555	1557	rBV	91983	81986	2.63%	0.306%
28	11.398	1579	1583	1585	rBV	841954	869498	27.86%	3.244%
29	11.421	1585	1587	1594	rVV	289838	331215	10.61%	1.236%
30	11.480	1594	1597	1604	rVB	49397	74988	2.40%	0.280%
31	11.657	1624	1627	1630	rVB2	60400	54155	1.73%	0.202%
32	11.904	1665	1669	1671	rBV2	37758	46674	1.50%	0.174%
33	11.933	1671	1674	1677	rVB2	40491	48520	1.55%	0.181%
34	12.015	1684	1688	1690	rBV2	34911	42841	1.37%	0.160%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.451	1759	1762	1765	rBV2	36989	40889	1.31%	0.153%
36	12.615	1787	1790	1799	rVV	294359	327065	10.48%	1.220%
37	12.827	1823	1826	1827	rBV	60398	50932	1.63%	0.190%
38	12.851	1827	1830	1835	rVB	300721	315639	10.11%	1.177%
39	12.980	1848	1852	1863	rVV	1936043	1897206	60.78%	7.077%
40	13.068	1863	1867	1873	rVB4	20446	40695	1.30%	0.152%
41	13.180	1879	1886	1891	rBV3	41702	84335	2.70%	0.315%
42	13.380	1916	1920	1923	rBV3	23548	31344	1.00%	0.117%
43	13.857	1998	2001	2007	rBV2	112376	147495	4.73%	0.550%
44	14.057	2030	2035	2038	rBV2	630069	756747	24.24%	2.823%
45	14.168	2051	2054	2058	rBV6	23839	42599	1.36%	0.159%
46	14.792	2158	2160	2163	rBV3	35548	37034	1.19%	0.138%
47	15.127	2213	2217	2225	rBV	115176	239721	7.68%	0.894%
48	15.439	2268	2270	2276	rVB	55943	60388	1.93%	0.225%
49	15.509	2279	2282	2287	rVV	77932	114258	3.66%	0.426%
50	15.568	2288	2292	2304	rVB	391442	601855	19.28%	2.245%

Sum of corrected areas: 26807294

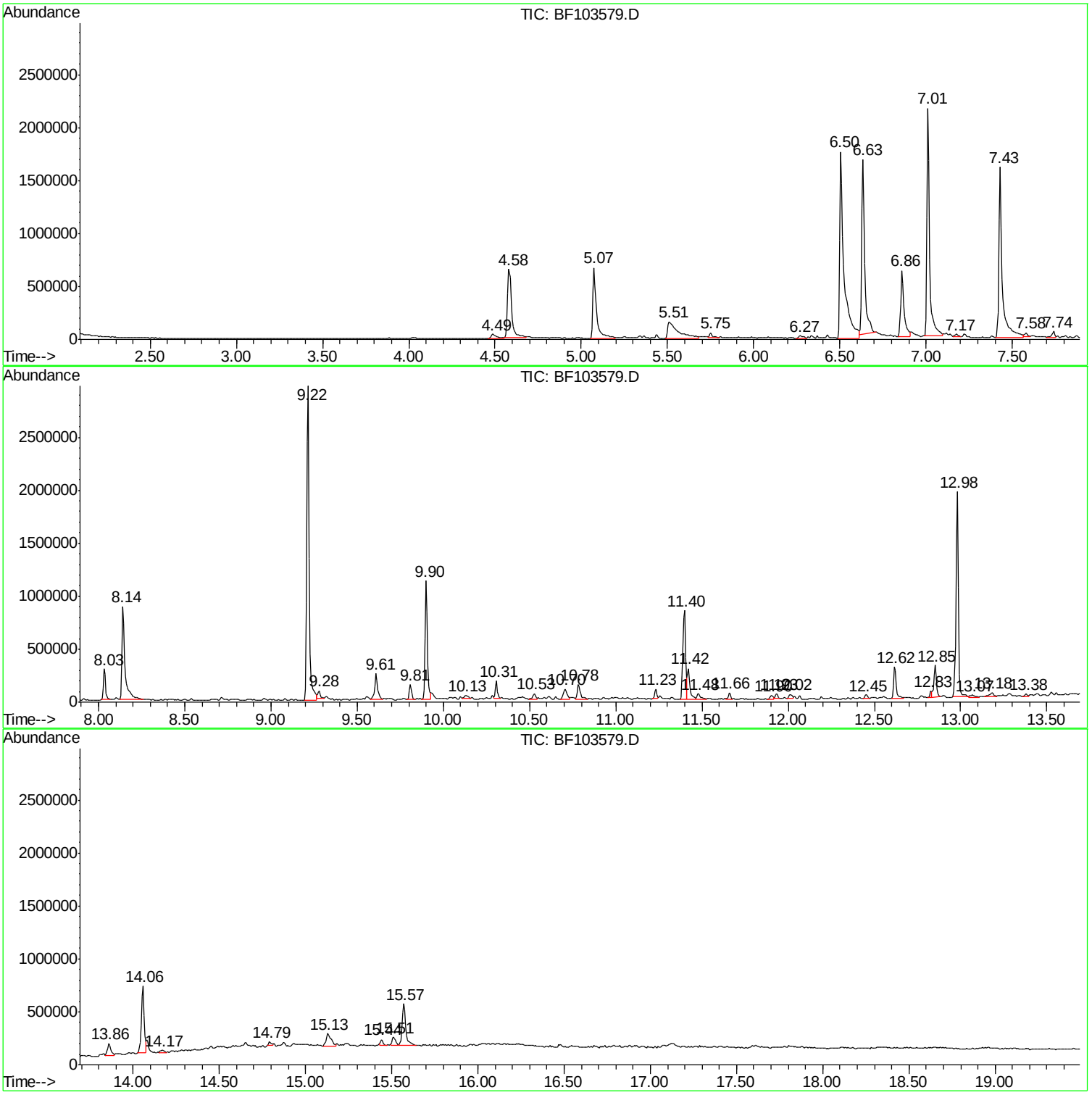
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

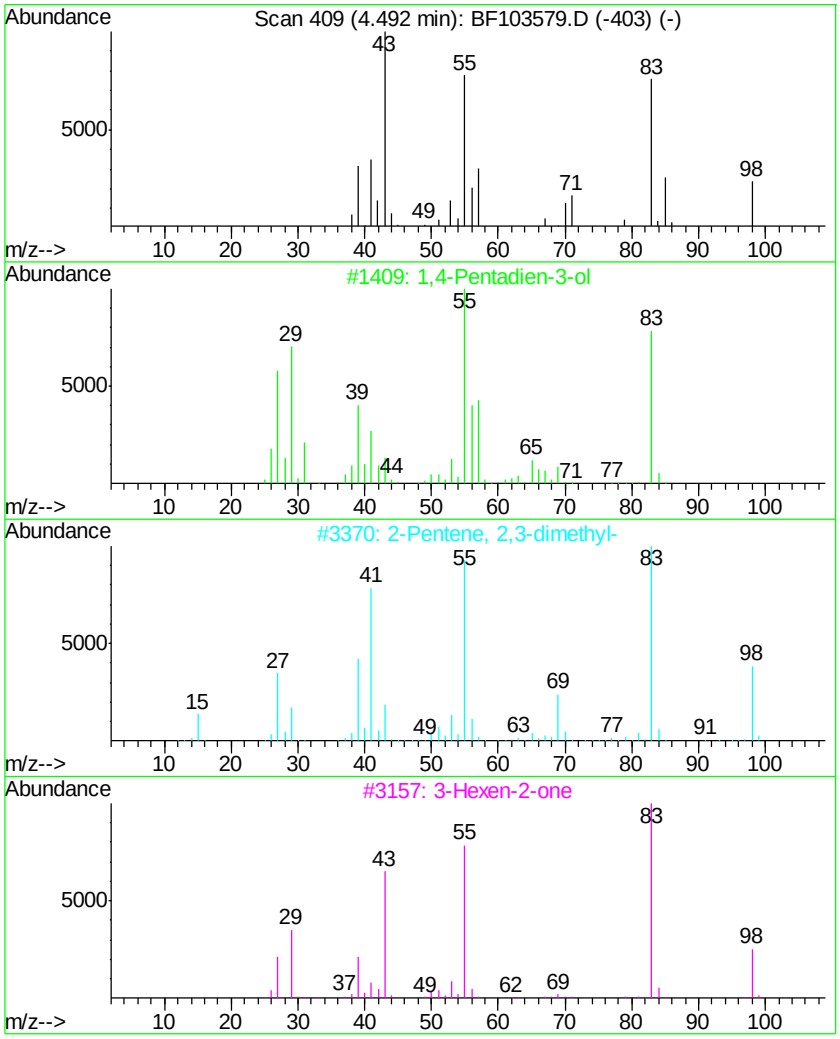
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

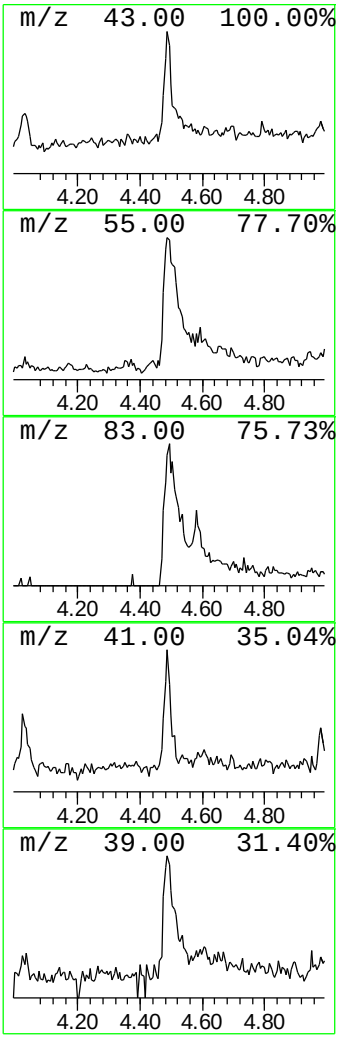
****

Peak Number 1 unknown4.49 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	2.32 ng	98301	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	49
2	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	47
3	3-Hexen-2-one	98	C6H10O	000763-93-9	46
4	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	46
5	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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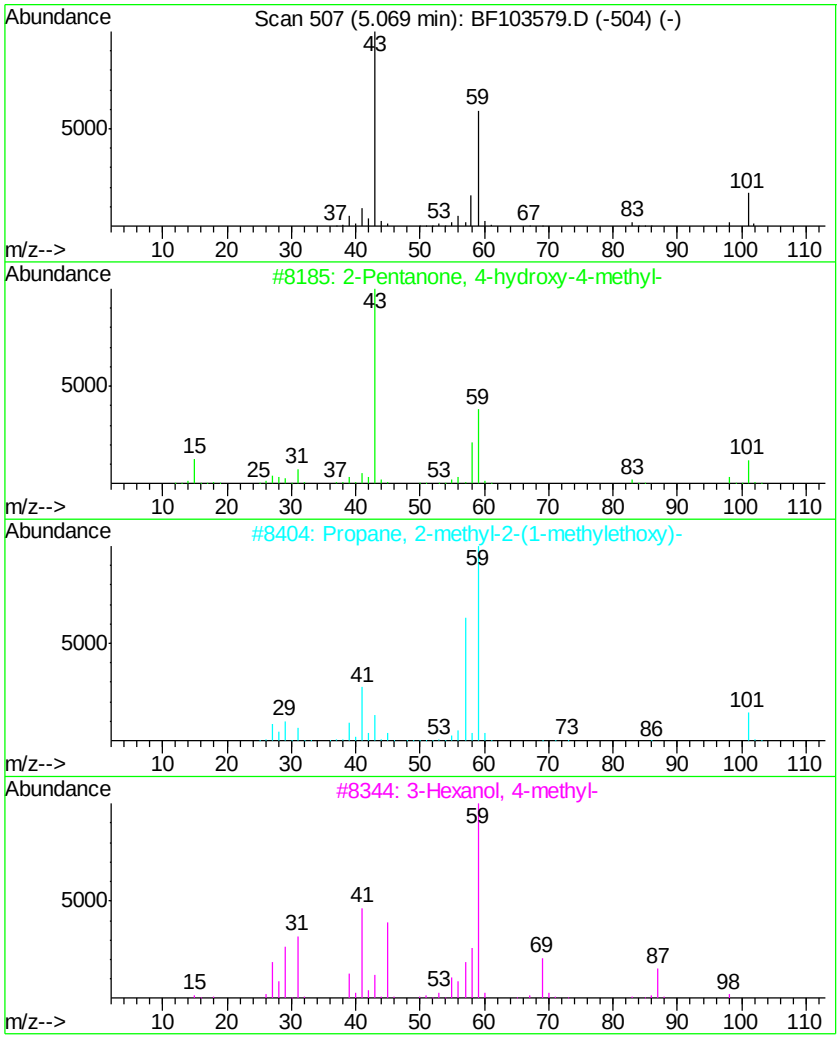
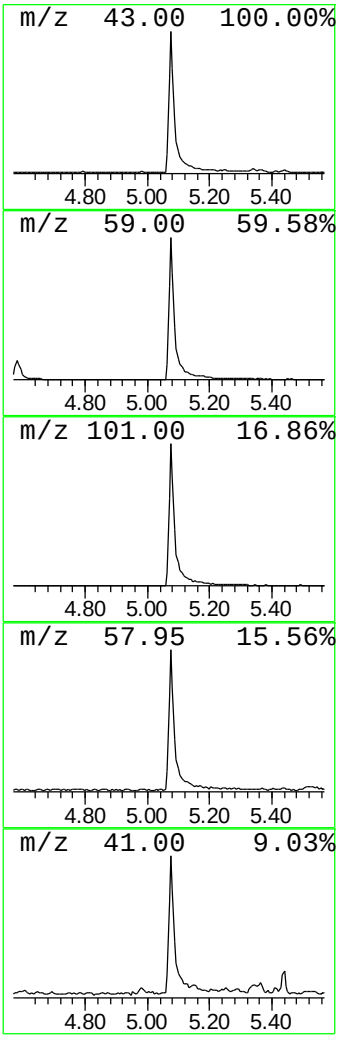
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	22.00 ng	931822	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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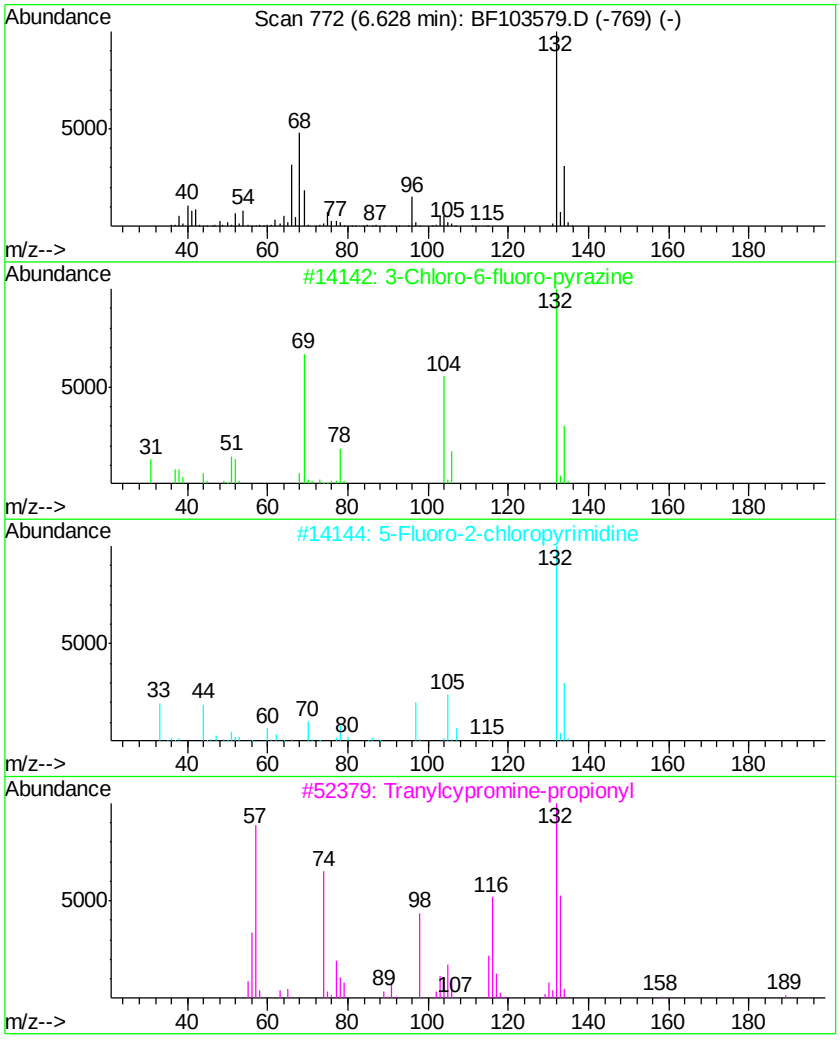
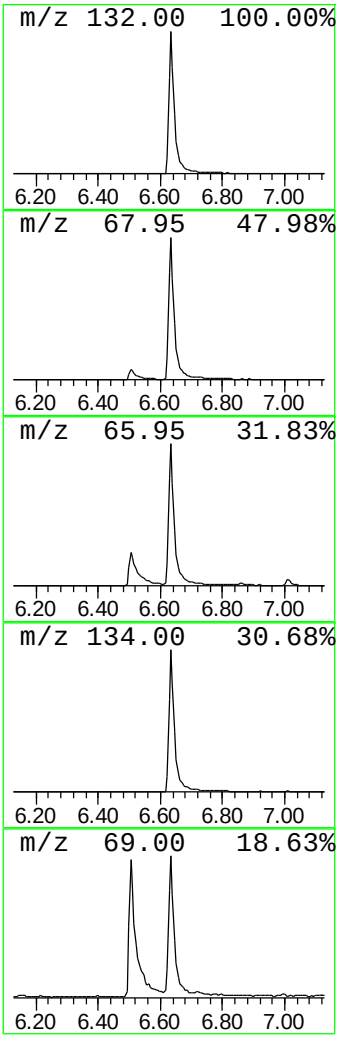
Peak Number 4 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	50.67 ng	2146260	1,4-Dichlorobenzene-d4	6.86

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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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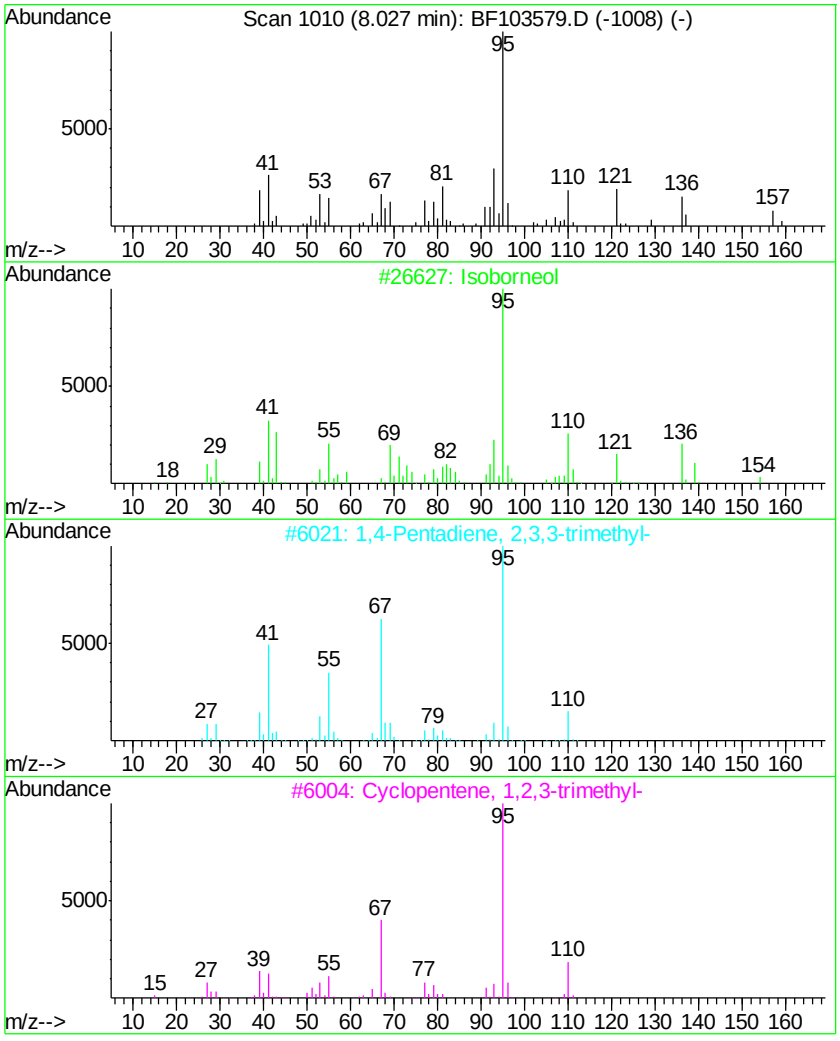
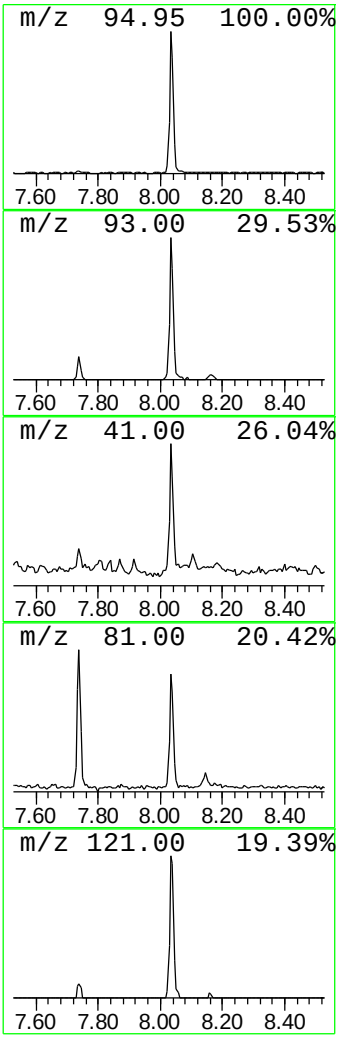
Peak Number 6 Isoborneol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.03	4.39 ng	257597	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoborneol	154	C10H18O	000124-76-5	72
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	64
3	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	64
4	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	58
5	Bornyl chloride	172	C10H17Cl	000464-41-5	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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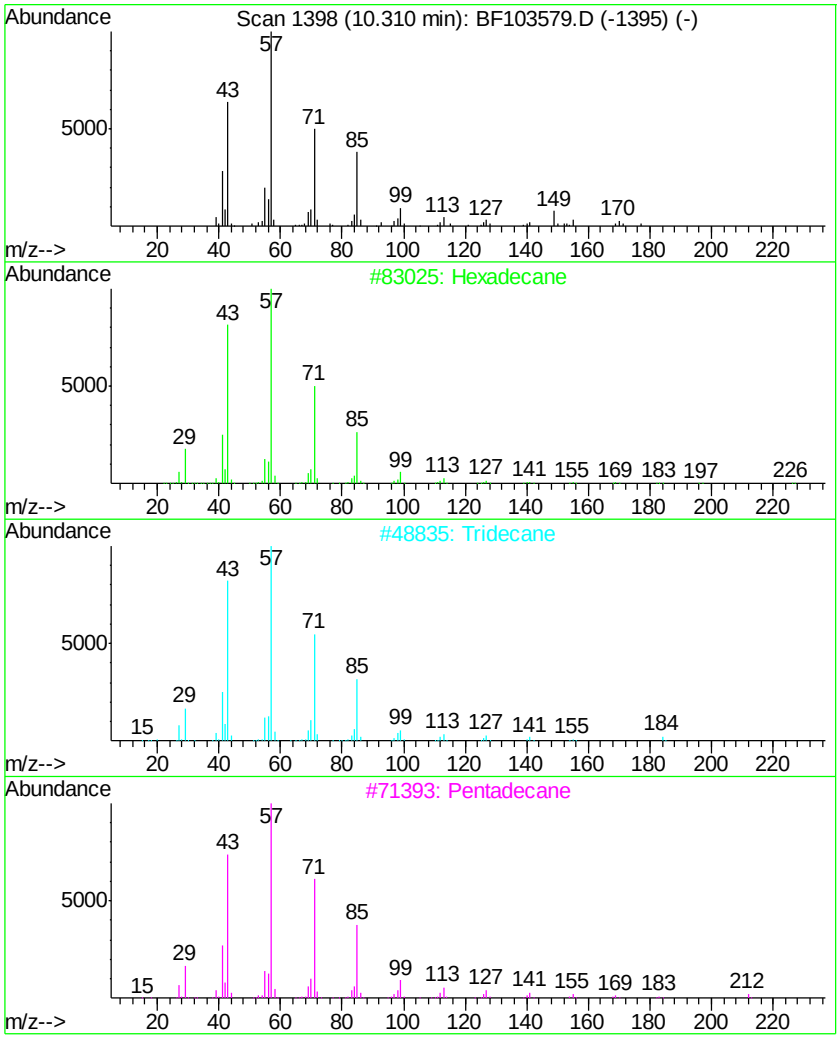
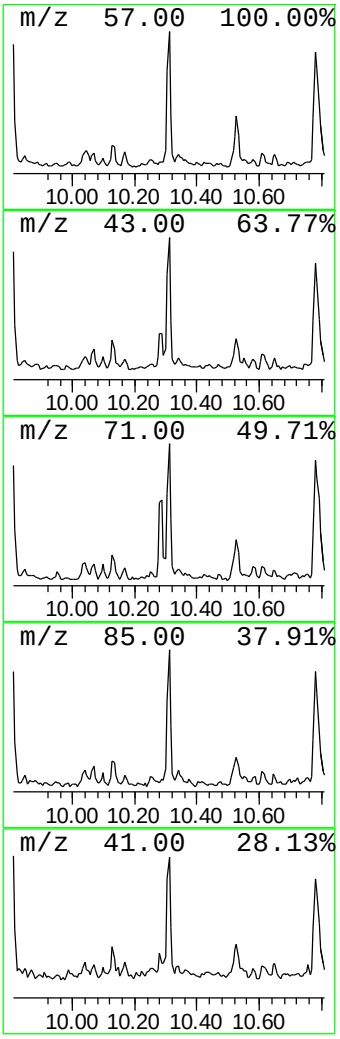
Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.31	2.36 ng	130803	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Pentadecane	212	C15H32	000629-62-9	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Dodecane	170	C12H26	000112-40-3	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

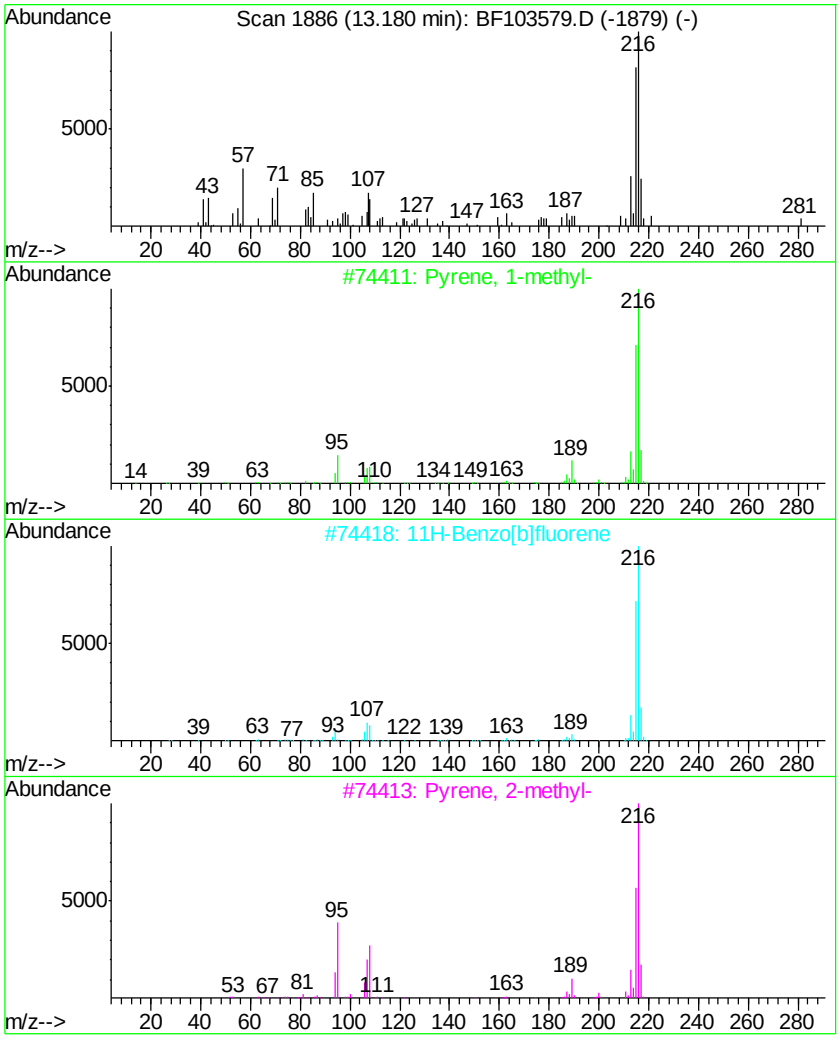
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

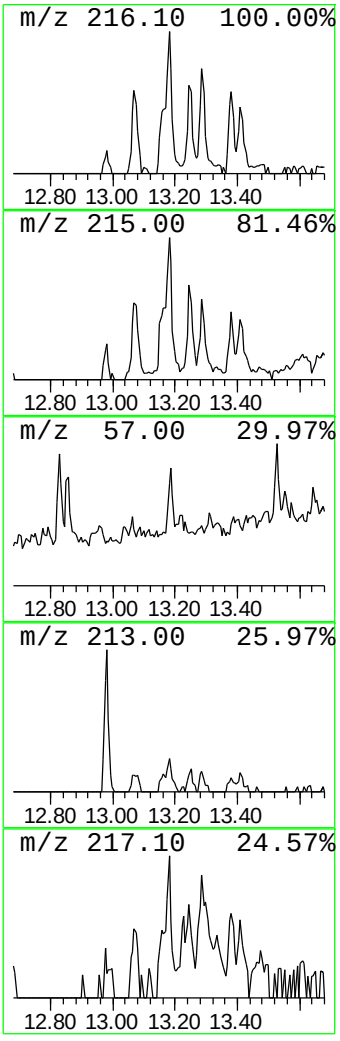
****

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	2.23 ng	84335	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	80
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	80
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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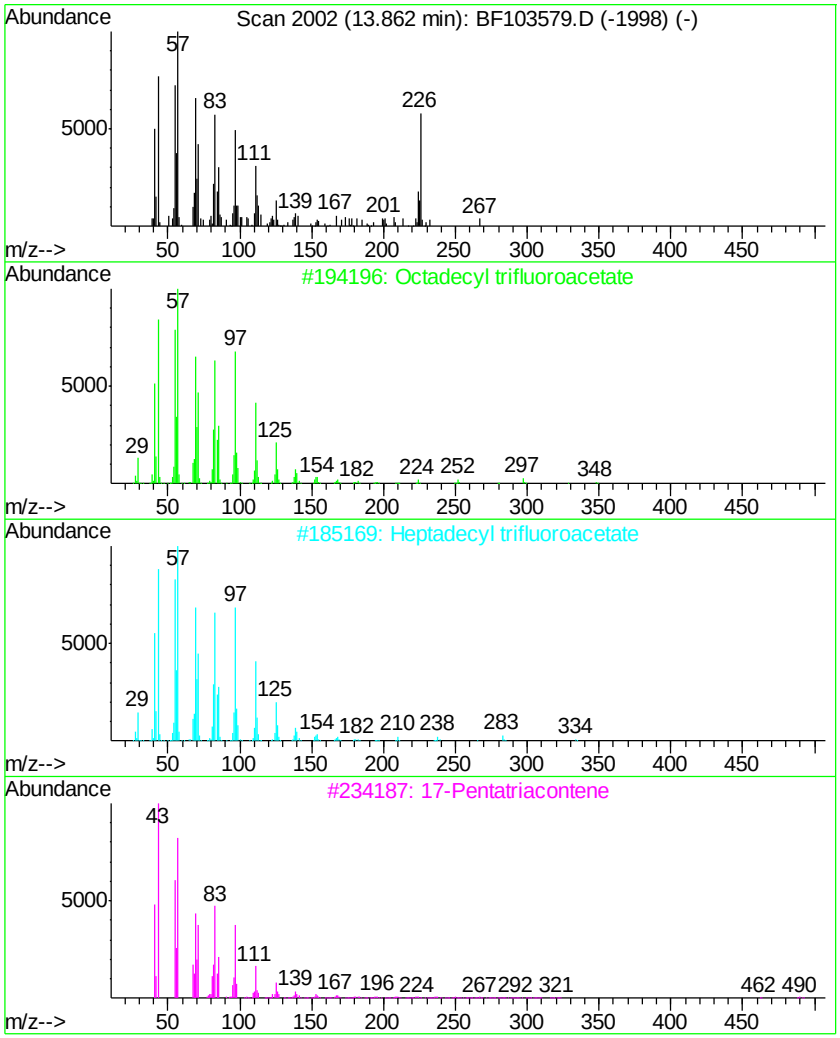
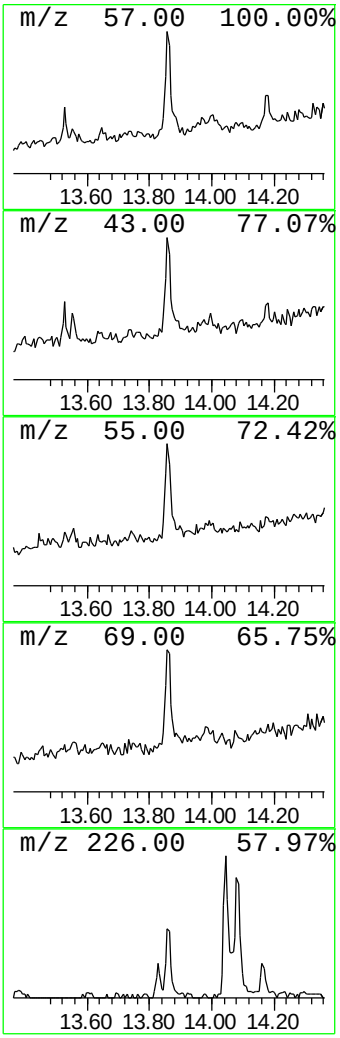
Peak Number 10 Octadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.90 ng	147495	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81
3	17-Pentatriacontene	491	C35H70	006971-40-0	81
4	1-Docosene	308	C22H44	001599-67-3	76
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031218\
Data File : BF103579.D
Acq On : 12 Mar 2018 13:59
Operator : SJ/JU
Sample : J1876-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-08-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
unknown4.49	4.49	2.3	ng	98301	1	6.86	847166	20.0
2-Pentanone, 4-hy...	5.07	22.0	ng	931822	1	6.86	847166	20.0
unknown6.63	6.63	50.7	ng	2146260	1	6.86	847166	20.0
Isoborneol	8.03	4.4	ng	257597	2	8.14	1172980	20.0
Hexadecane	10.31	2.4	ng	130803	3	9.90	1108590	20.0
Pyrene, 1-methyl-	13.18	2.2	ng	84335	5	14.06	756747	20.0
Octadecyl trifluo...	13.86	3.9	ng	147495	5	14.06	756747	20.0