LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097643.D
Acq On : 12 Aug 2017 19:48
Operator : SJ/JU
Sample : I4705-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-B-COMP

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-BF081117.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	4.740	516	519	535	rBV2	92307	250533	10.06%	1.128%
2	5.416	629	634	658	rBV	1229174	2320712	93.22%	10.450%
3	7.057	908	913	926	rBV	1621880	2459332	98.79%	11.074%
4	7.157	926	930	942	rVB	1668113	2489537	100.00%	11.210%
5	7.498	984	988	1002	rBV	498441	712189	28.61%	3.207%
6	7.734	1024	1028	1054	rVB	1194290	1716439	68.95%	7.729%
7	8.410	1138	1143	1165	rBV	1049401	1445886	58.08%	6.511%
8	9.528	1329	1333	1351	rBV	721388	969655	38.95%	4.366%
9	11.304	1629	1635	1650	rBV	1858512	2316152	93.04%	10.429%
10	11.416	1650	1654	1661	rBV3	13662	30570	1.23%	0.138%
11	11.992	1747	1752	1759	rBV	360104	441142	17.72%	1.986%
12	12.351	1808	1813	1818	rBV2	628375	807194	32.42%	3.635%
13	13.204	1951	1958	1963	rBV	36831	48610	1.95%	0.219%
14	13.557	2005	2018	2023	rBV3	12124	27110	1.09%	0.122%
15	13.645	2028	2033	2047	rBV	827874	1169383	46.97%	5.266%
16	13.974	2084	2089	2091	rBV	52417	68068	2.73%	0.306%
17	14.704	2209	2213	2216	rBV	32505	36545	1.47%	0.165%
18	14.745	2216	2220	2234	rVB2	484535	692452	27.81%	3.118%
19	14.886	2240	2244	2248	rBV3	16578	26271	1.06%	0.118%
20	15.533	2350	2354	2357	rBV	22208	26179	1.05%	0.118%
21	15.745	2386	2390	2397	rVB5	18773	29276	1.18%	0.132%
22	16.527	2520	2523	2526	rVV2	42873	57626	2.31%	0.259%
23	16.557	2526	2528	2535	rVB	56196	63436	2.55%	0.286%
24	16.857	2574	2579	2583	rBV2	49946	63753	2.56%	0.287%
25	17.104	2616	2621	2628	rVB	1251887	1458964	58.60%	6.569%
26	17.298	2649	2654	2656	rBV4	17511	25596	1.03%	0.115%
27	17.327	2656	2659	2665	rVB7	19344	27954	1.12%	0.126%
28	18.304	2821	2825	2830	rBV	49868	62936	2.53%	0.283%
29	18.362	2830	2835	2840	rBV	76485	144368	5.80%	0.650%
30	18.445	2844	2849	2854	rVV	482711	635130	25.51%	2.860%
31	18.515	2858	2861	2866	rVB3	26596	32942	1.32%	0.148%
32	18.574	2868	2871	2877	rVV2	37922	46344	1.86%	0.209%
33	18.727	2894	2897	2902	rBV2	16733	26249	1.05%	0.118%
34	18.774	2903	2905	2912	rVB8	17540	29648	1.19%	0.133%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.709	3060	3064	3068	rBV	169142	239332	9.61%	1.078%
36	19.827	3081	3084	3090	rBV	33624	45731	1.84%	0.206%
37	20.003	3110	3114	3118	rBV	108648	138497	5.56%	0.624%
38	20.062	3120	3124	3127	rBV	123959	129393	5.20%	0.583%
39	20.109	3129	3132	3138	rBV	408172	495265	19.89%	2.230%
40	20.215	3147	3150	3156	rVB8	30933	40697	1.63%	0.183%
41	20.527	3200	3203	3206	rBV5	25928	46404	1.86%	0.209%
42	20.715	3233	3235	3239	rBV4	24498	32193	1.29%	0.145%
43	21.139	3306	3307	3310	rBV2	23091	25516	1.02%	0.115%
44	21.215	3317	3320	3324	rVB6	24583	32500	1.31%	0.146%
45	21.339	3336	3341	3346	rBV2	73474	114457	4.60%	0.515%
46	21.444	3355	3359	3363	rBV7	36104	75871	3.05%	0.342%
47	22.991	3619	3622	3625	rBV5	20576	34321	1.38%	0.155%

Sum of corrected areas: 22208358

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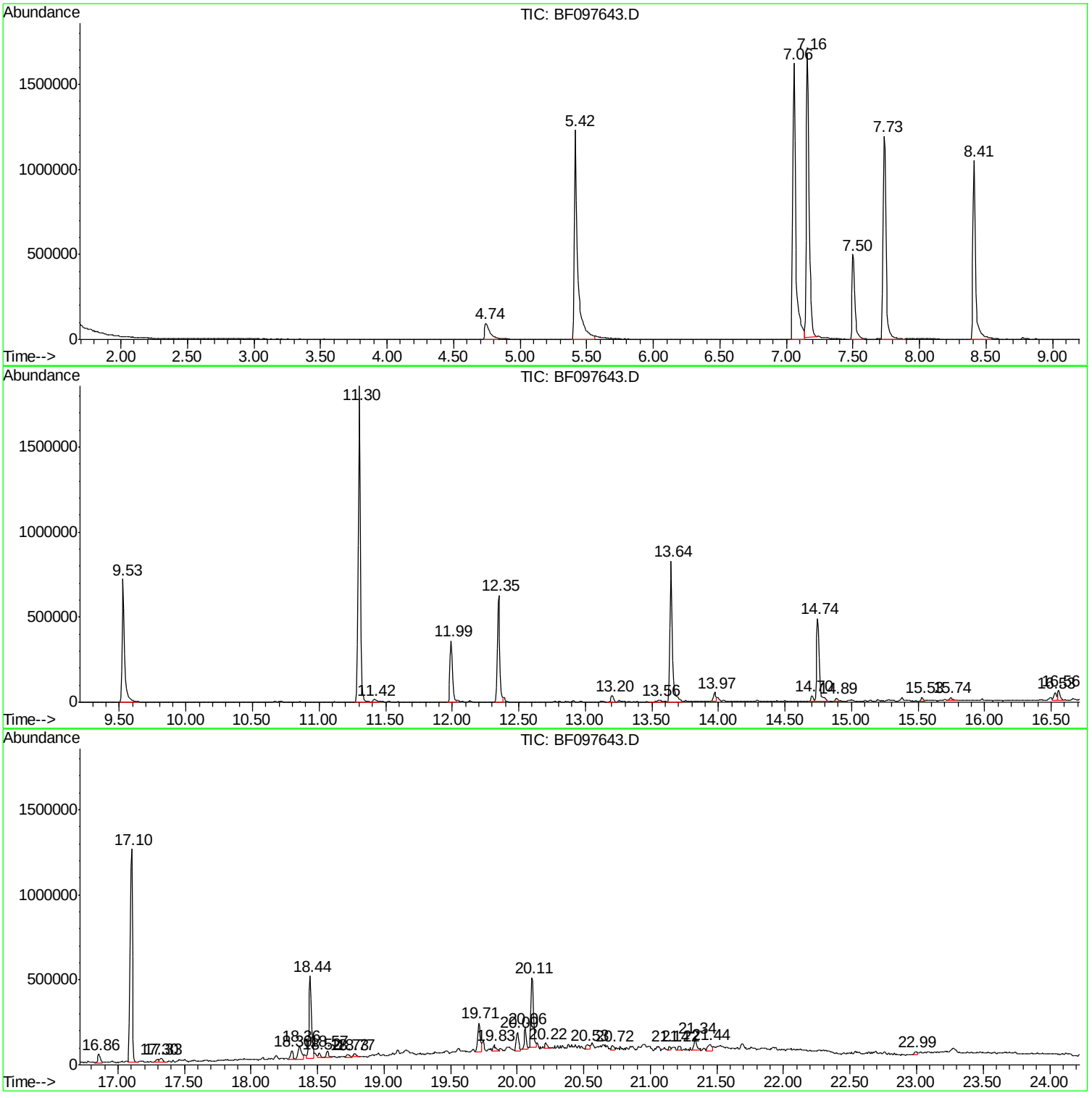
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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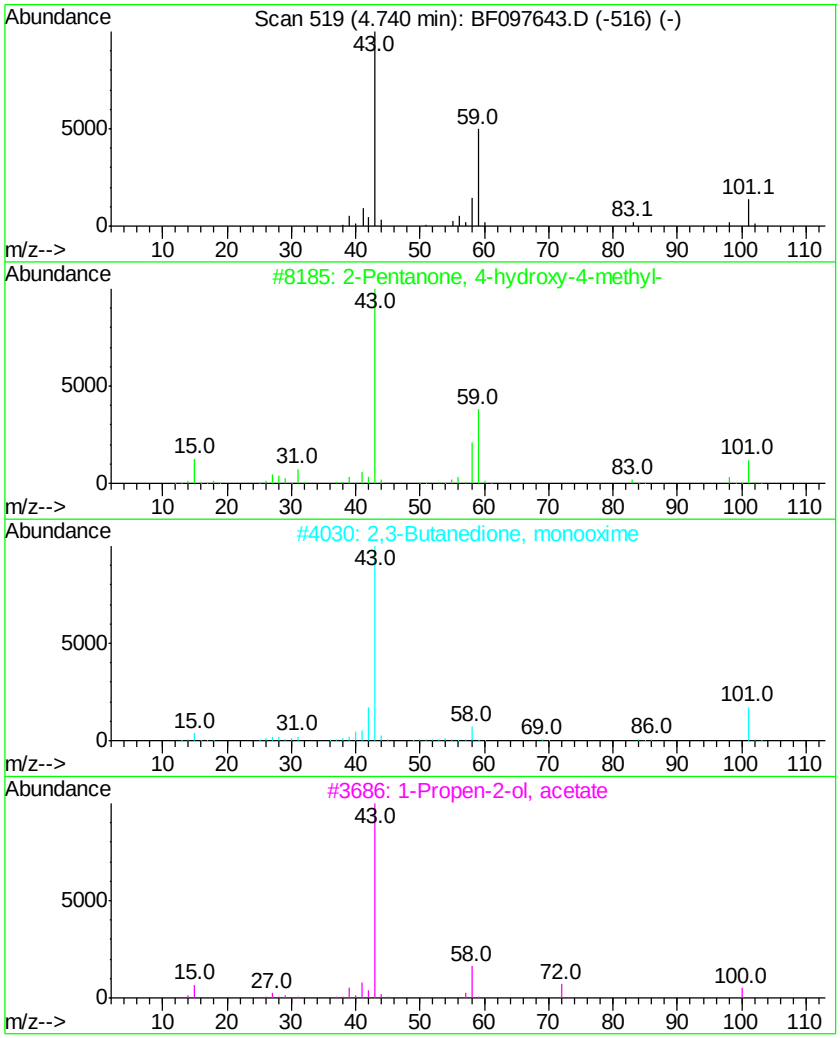
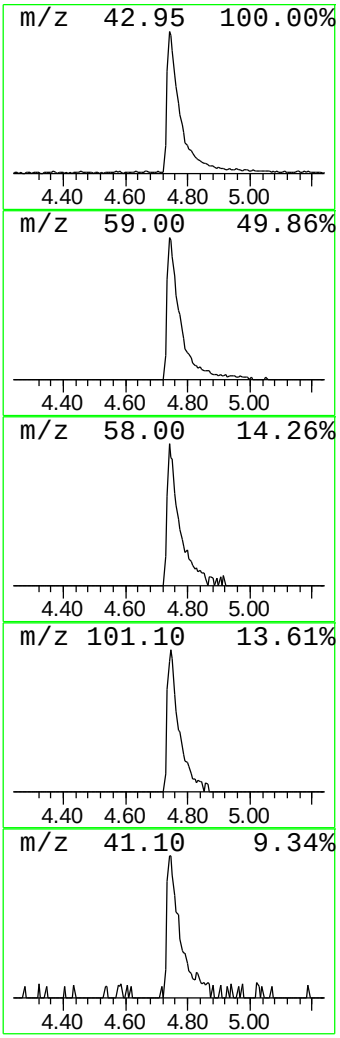
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	7.04 ng	250533	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Instrument : BNA_F
ClientSampleId : SP-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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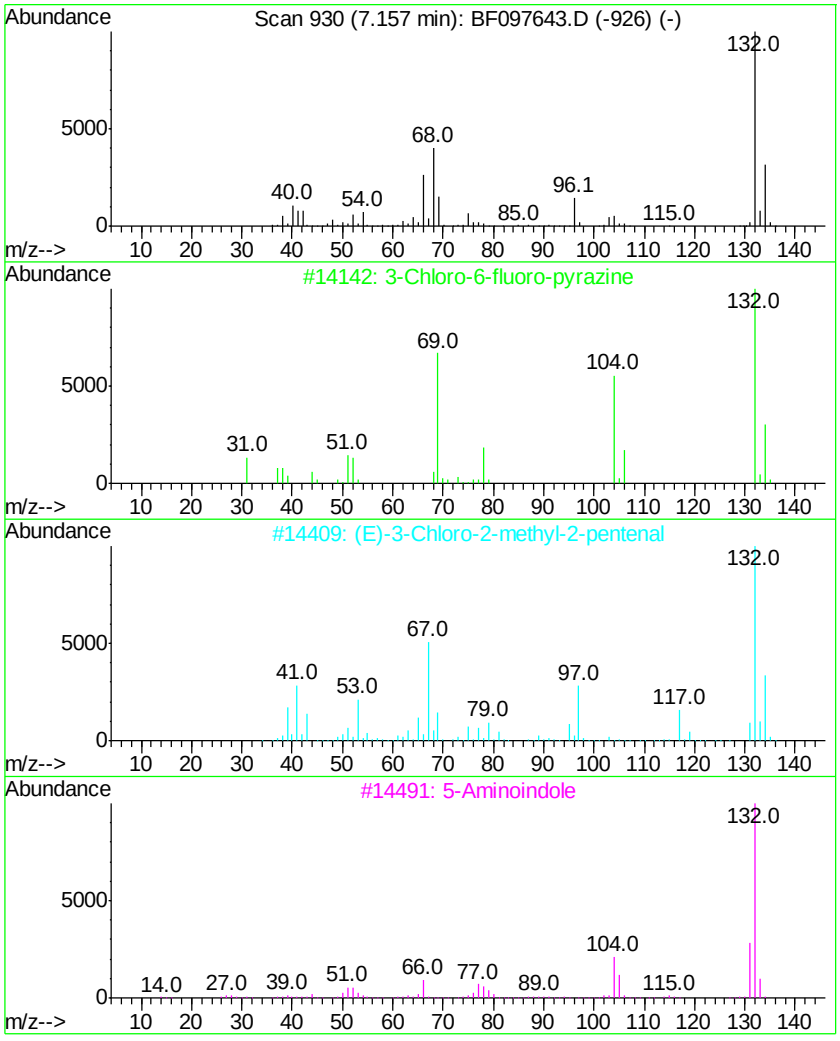
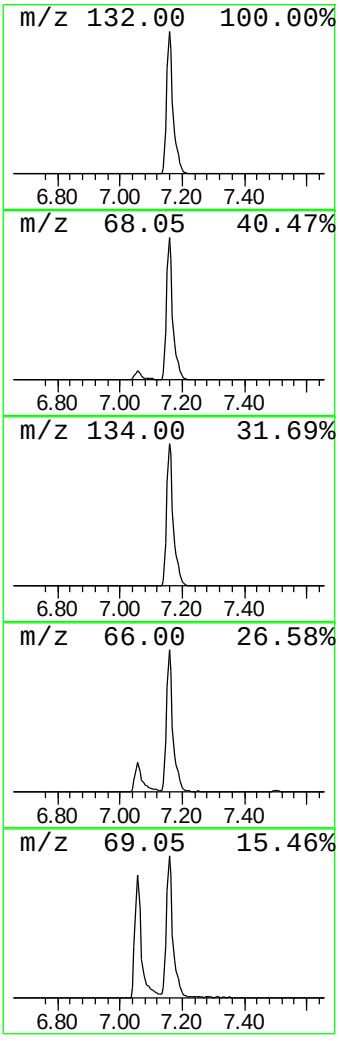
Peak Number 2 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	69.91 ng	2489540	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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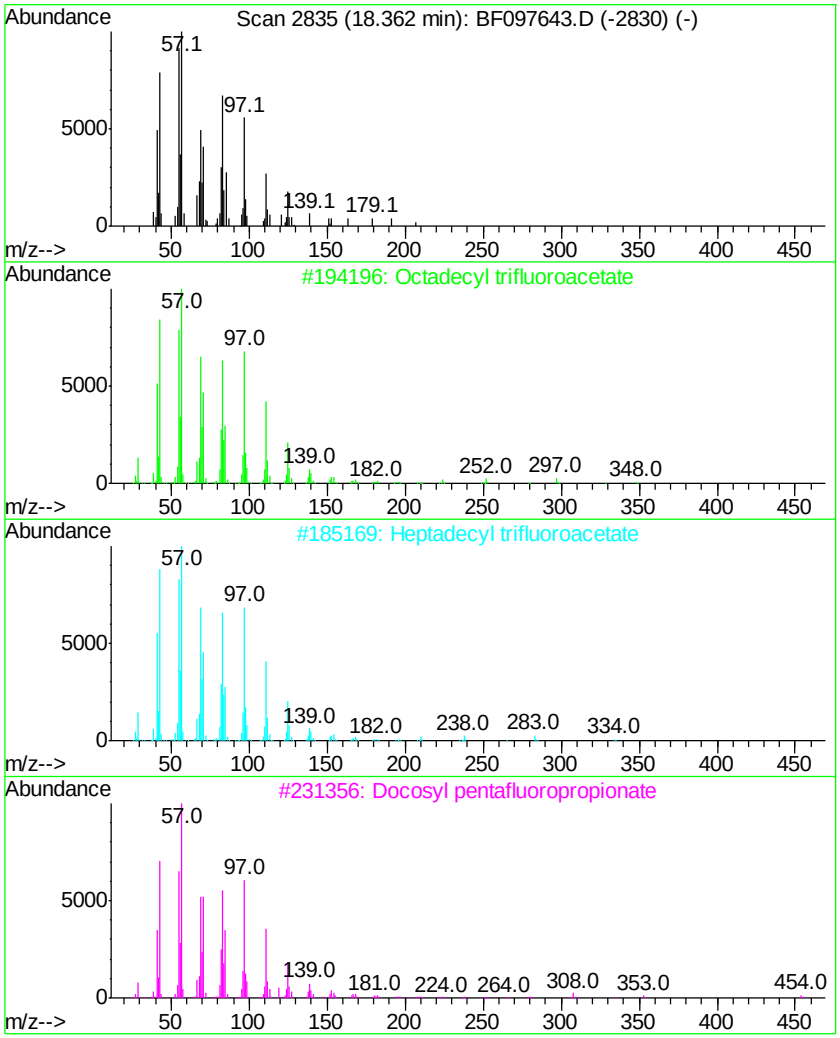
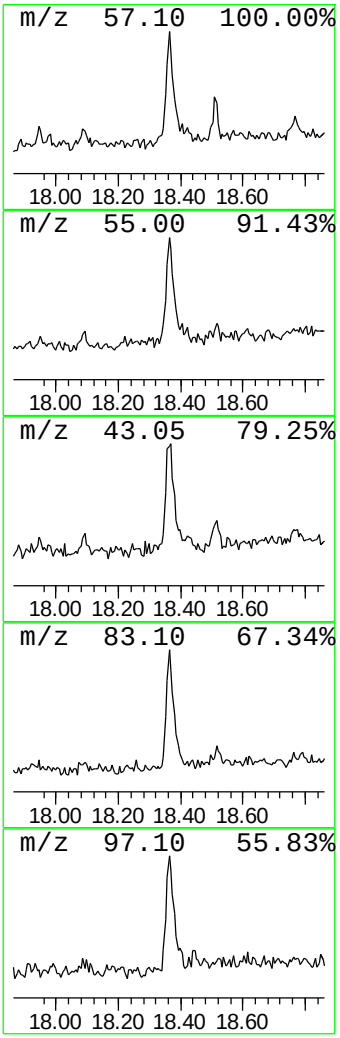
Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	4.55 ng	144368	Chrysene-d12	18.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	83
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	83





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

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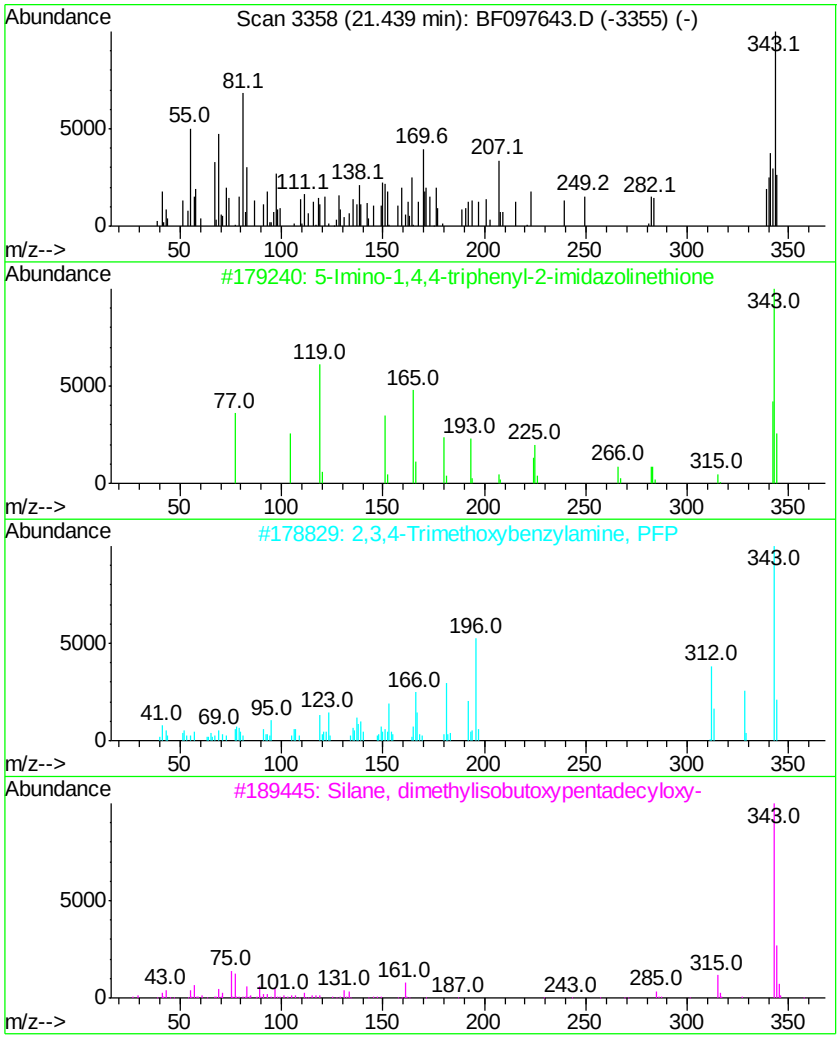
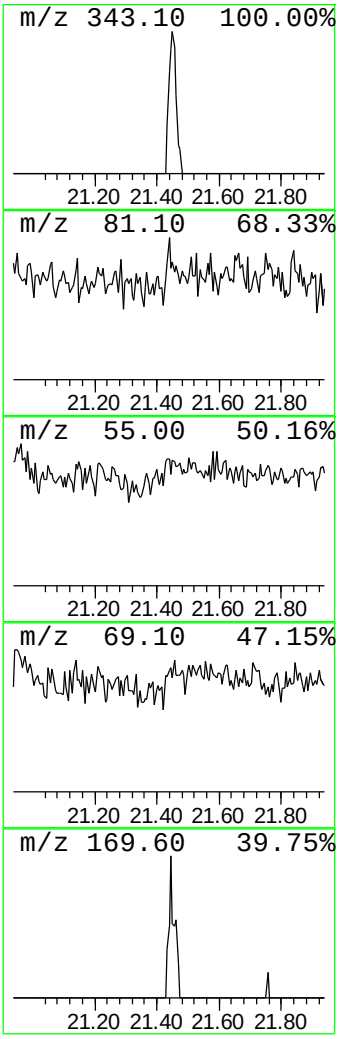
Peak Number 7 unknown21.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	3.06 ng	75871	Perylene-d12	20.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Imino-1,4,4-triphenyl-2-imidaz...	343	C21H17N3S	052460-97-6	43
2	2,3,4-Trimethoxybenzylamine, PFP	343	C13H14F5NO4	1000072-05-4	12
3	Silane, dimethylisobutoxypentade...	358	C21H46O2Si	1000346-77-4	10
4	Silane, dimethyl(3-methylpentylo...	358	C21H46O2Si	1000347-70-2	10
5	2,4,5-Trimethoxybenzylamine, PFP	343	C13H14F5NO4	1000072-05-8	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.74	7.0	ng	250533	1	7.50	712189	20.0
unknown7.16	7.16	69.9	ng	2489540	1	7.50	712189	20.0
Octadecyl trifluo...	18.36	4.5	ng	144368	5	18.44	635130	20.0
unknown21.44	21.44	3.1	ng	75871	6	20.12	495265	20.0