LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097885.D
Acq On : 19 Aug 2017 18:11
Operator : SJ/JU
Sample : I4659-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF081517.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	4.969	485	490	503	rVB	499818	829889	17.29%	2.150%
2	5.375	553	559	562	rBV	3530725	4358346	90.83%	11.289%
3	6.404	727	734	737	rBV	3766596	4629801	96.48%	11.992%
4	6.534	750	756	759	rBV	3821758	4372421	91.12%	11.326%
5	6.763	791	795	798	rBV	921630	818382	17.05%	2.120%
6	6.922	817	822	825	rBV	3265936	3303945	68.85%	8.558%
7	7.328	885	891	894	rBV	2719956	3001758	62.55%	7.775%
8	8.045	1008	1013	1016	rBV	1224827	1123078	23.40%	2.909%
9	9.122	1190	1196	1199	rBV	4382450	4798604	100.00%	12.429%
10	9.510	1258	1262	1266	rBV	698549	576098	12.01%	1.492%
11	9.792	1306	1310	1314	rBV	1324892	1215434	25.33%	3.148%
12	10.586	1439	1445	1448	rBV	2532125	2674363	55.73%	6.927%
13	10.704	1462	1465	1474	rBV	92100	98745	2.06%	0.256%
14	11.151	1538	1541	1543	rBV	67391	50179	1.05%	0.130%
15	11.275	1558	1562	1565	rBV	1413980	1157344	24.12%	2.998%
16	11.739	1636	1641	1644	rBV2	37651	54570	1.14%	0.141%
17	12.869	1827	1833	1836	rBV	3338759	3605123	75.13%	9.338%
18	13.757	1981	1984	1991	rBV	228893	237573	4.95%	0.615%
19	13.904	2005	2009	2012	rBV	825708	745382	15.53%	1.931%
20	14.757	2151	2154	2159	rVB	64448	61383	1.28%	0.159%
21	15.327	2246	2251	2256	rBV	554463	648112	13.51%	1.679%
22	15.792	2326	2330	2335	rBV2	46497	74432	1.55%	0.193%
23	16.274	2408	2412	2418	rVB2	34791	54336	1.13%	0.141%
24	16.839	2501	2508	2513	rBV3	31564	65176	1.36%	0.169%
25	17.498	2615	2620	2628	rVB4	22880	52305	1.09%	0.135%

Sum of corrected areas: 38606779

LSC Report - Integrated Chromatogram

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Instrument : BNA_F
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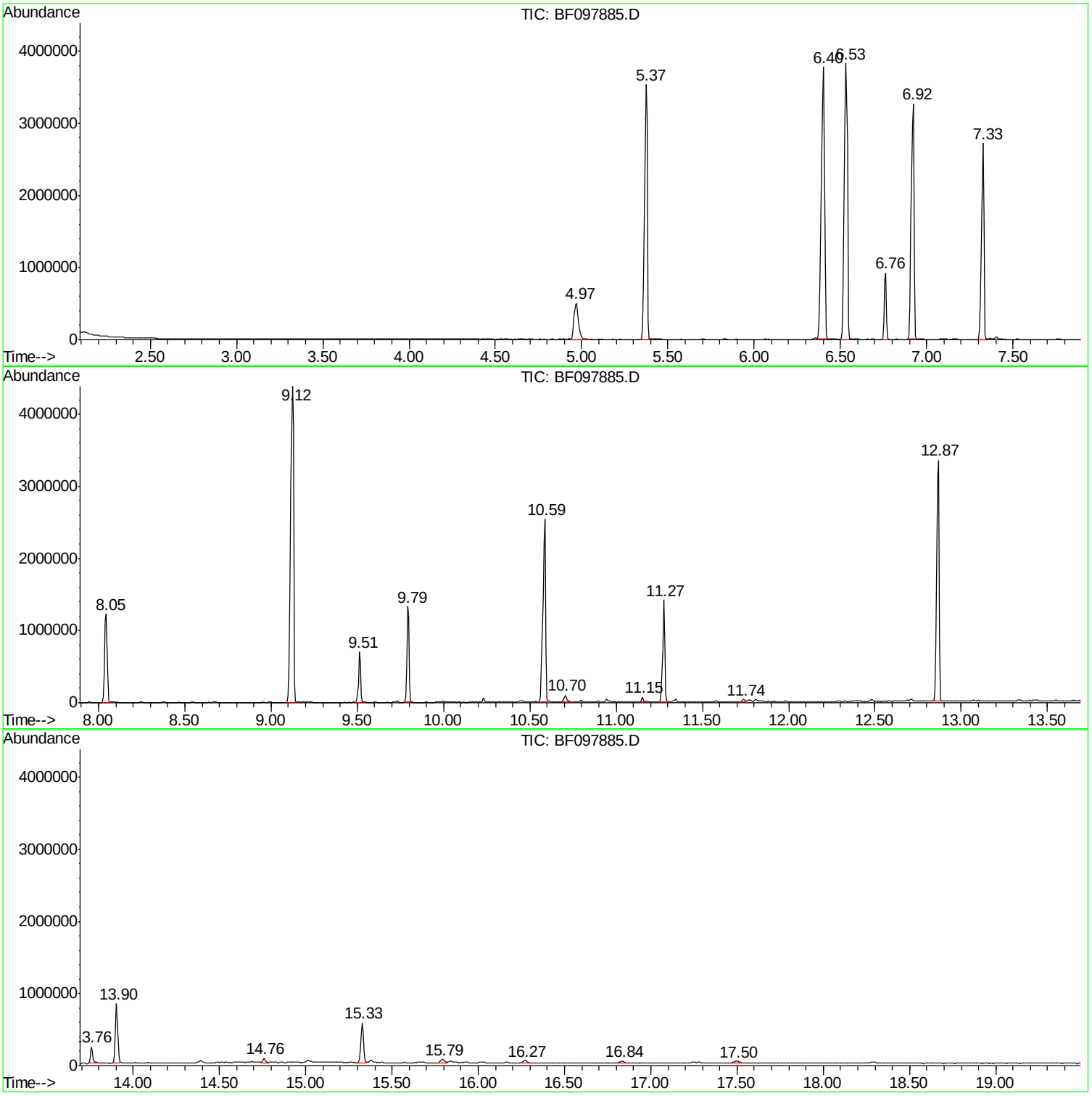
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097885.D
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Sample : I4659-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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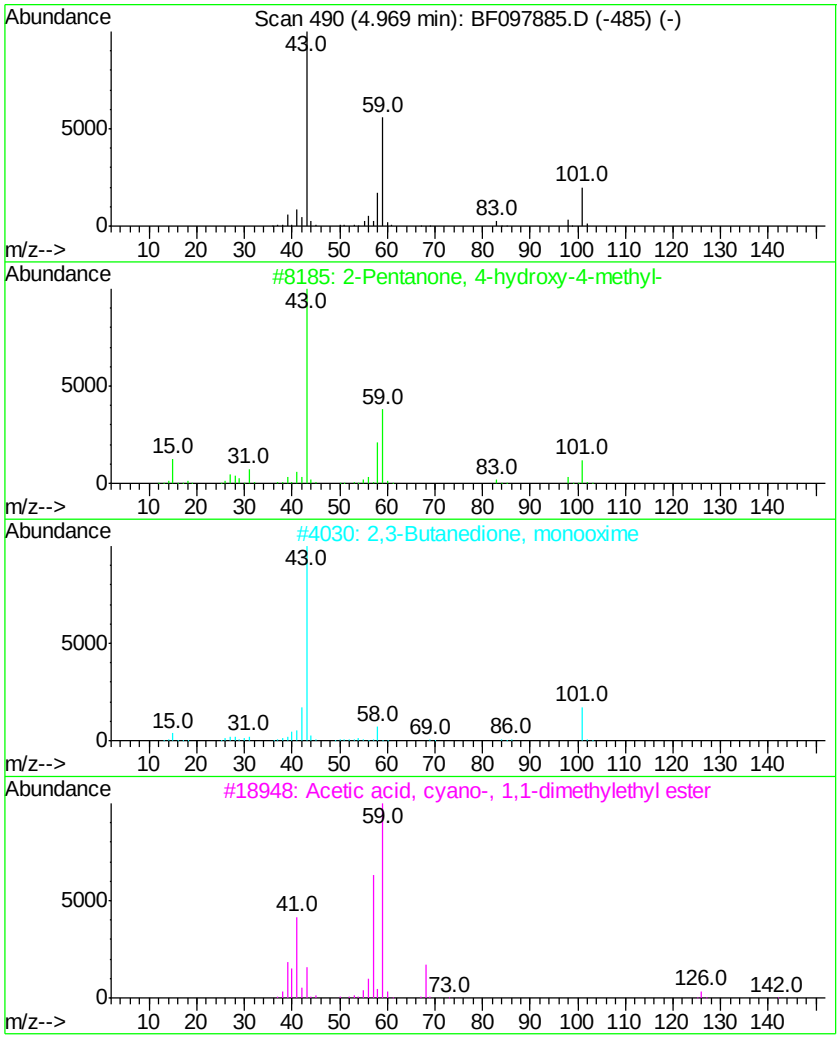
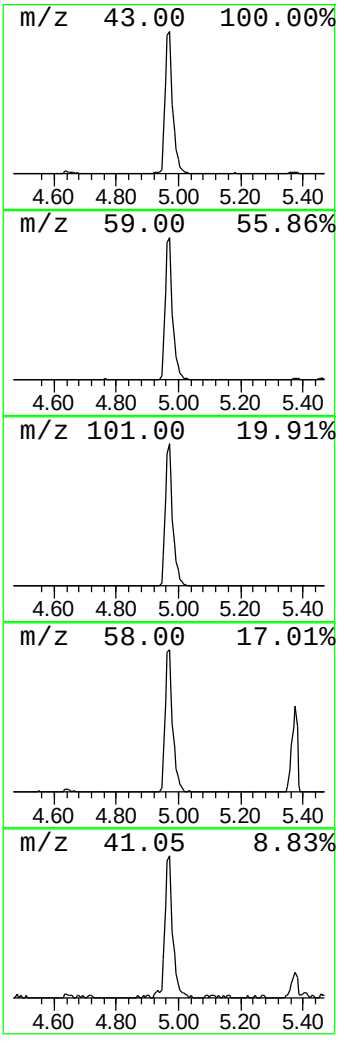
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	20.28 ng	829889	1,4-Dichlorobenzene-d4	6.76

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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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ClientSampleId : WC-1

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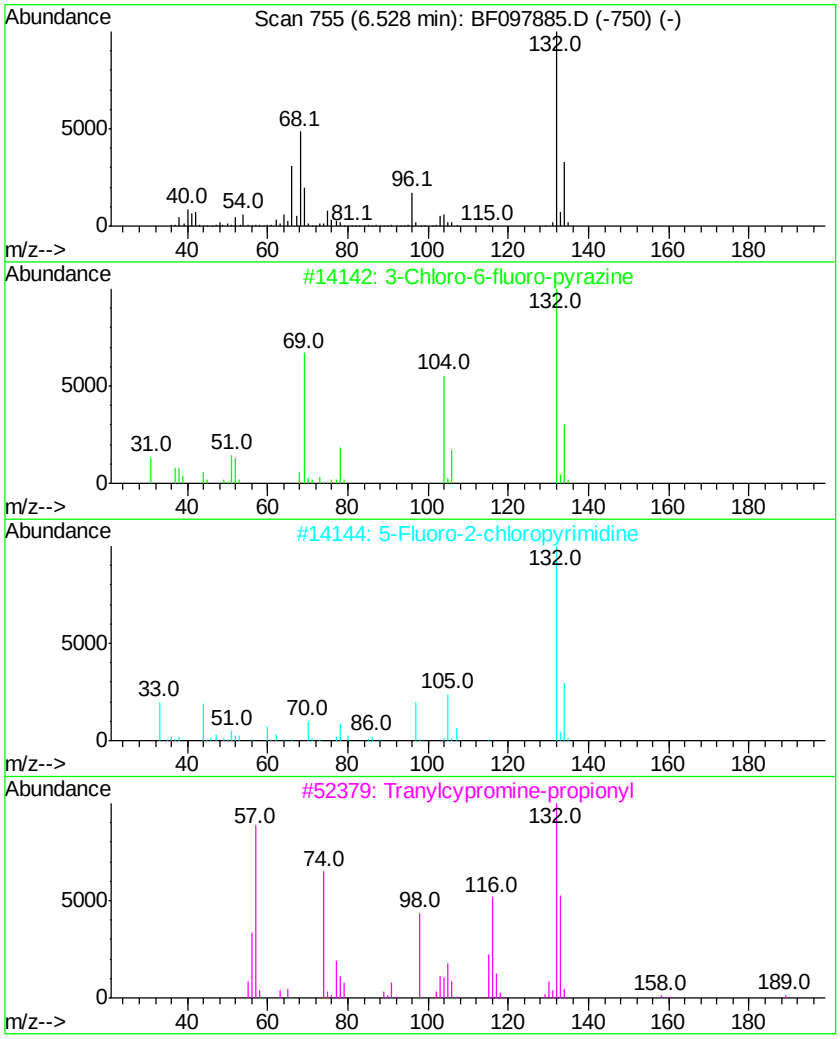
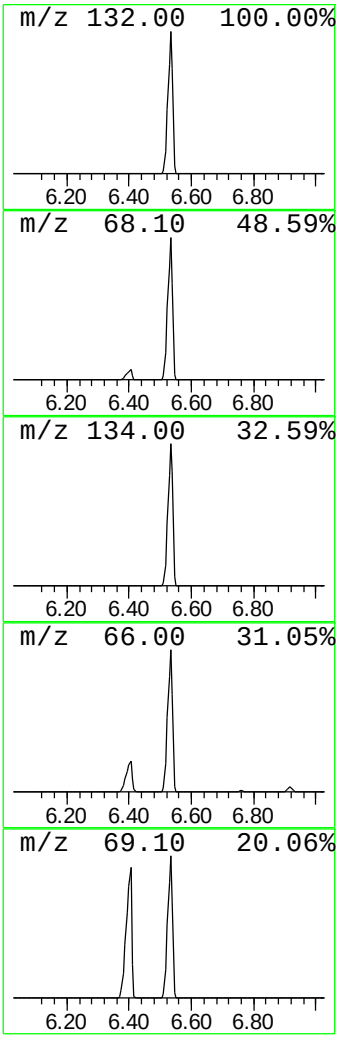
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	106.86 ng	4372420	1,4-Dichlorobenzene-d4	6.76

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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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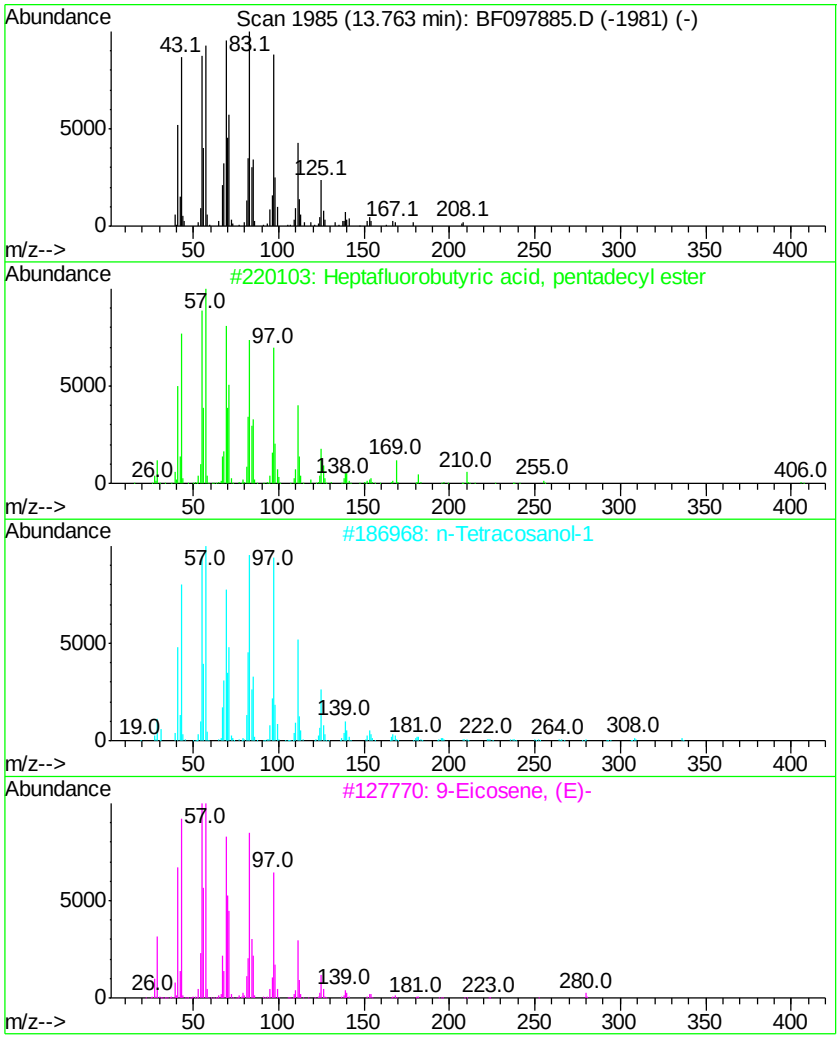
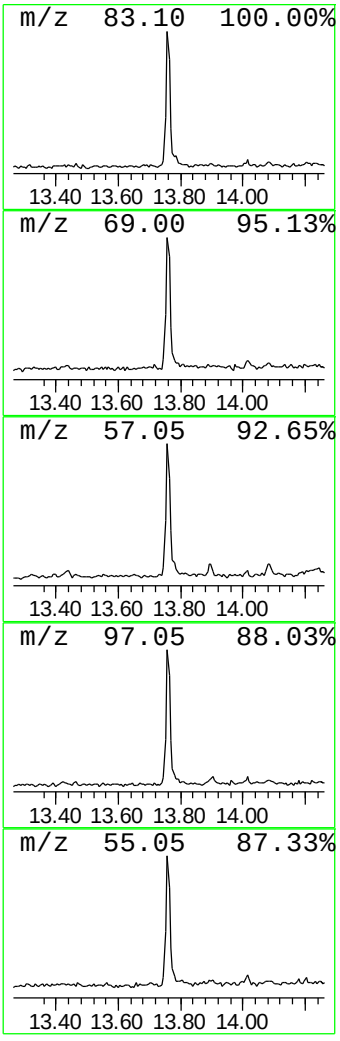
Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.37 ng	237573	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Instrument : BNA_F
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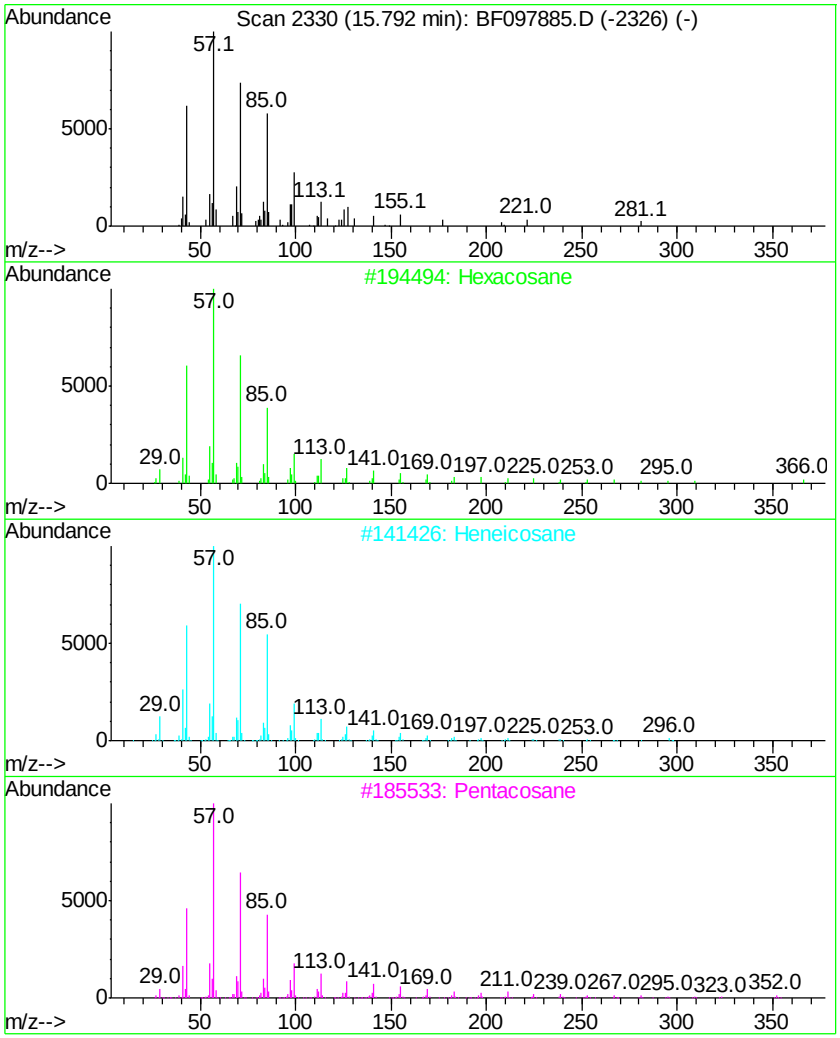
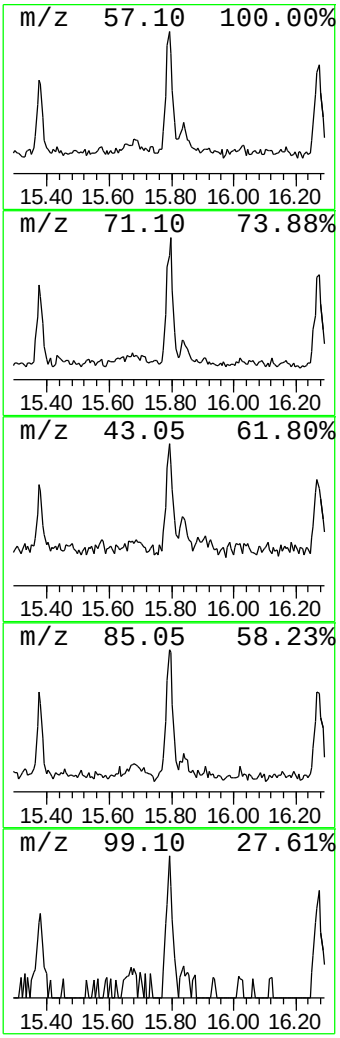
Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.30 ng	74432	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	80





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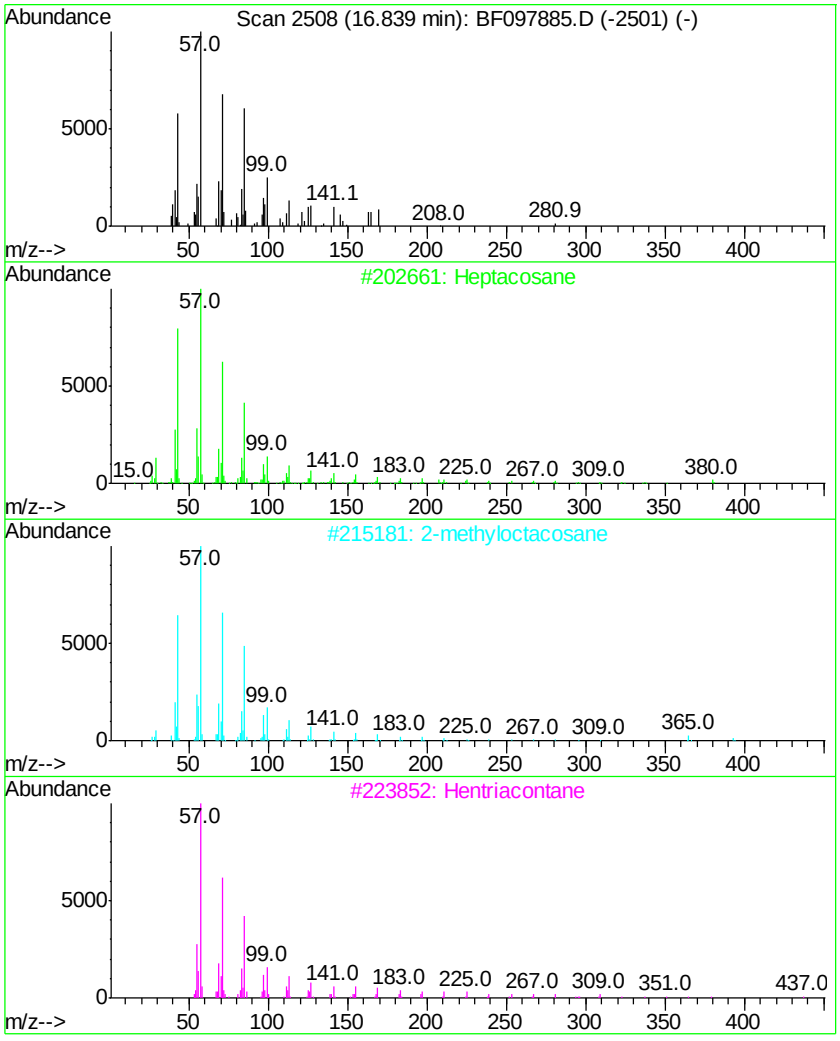
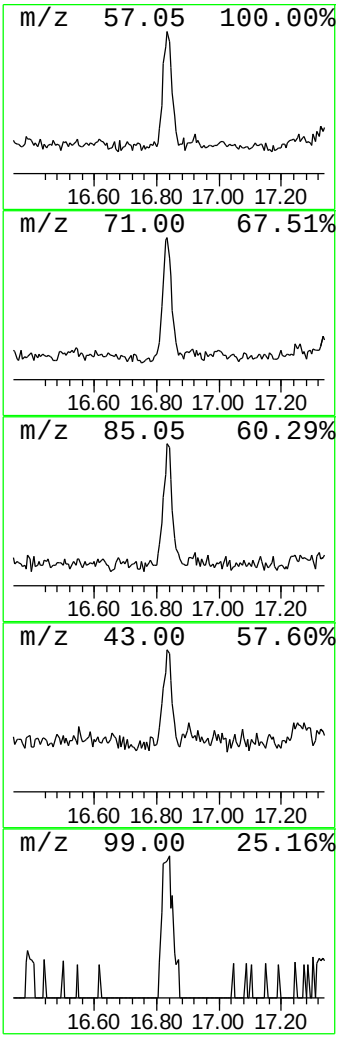
Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.01 ng	65176	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	86
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Octacosane	394	C28H58	000630-02-4	80
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	20.3	ng	829889	1	6.76	818382	20.0
unknown6.53	6.53	106.9	ng	4372420	1	6.76	818382	20.0
Heptafluorobutyri...	13.76	6.4	ng	237573	5	13.90	745382	20.0
Hexacosane	15.79	2.3	ng	74432	6	15.33	648112	20.0
Heptacosane	16.84	2.0	ng	65176	6	15.33	648112	20.0