LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099083.D
Acq On : 4 Oct 2017 22:52
Operator : SJ/JU
Sample : I5644-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-13-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-BF092317.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	2.175	10	15	23	rVB	170118	237348	6.93%	0.781%
2	2.999	150	155	165	rVB	40946	67331	1.97%	0.222%
3	4.475	403	406	414	rBV	95176	107947	3.15%	0.355%
4	5.099	508	512	527	rVB	395554	547057	15.98%	1.800%
5	5.493	573	579	582	rBV	3095968	3253321	95.02%	10.705%
6	6.498	744	750	753	rBV	2880748	3286825	96.00%	10.815%
7	6.640	768	774	777	rBV	3043785	3338380	97.50%	10.985%
8	6.863	808	812	816	rBV	983235	774107	22.61%	2.547%
9	7.022	834	839	842	rBV	2813017	2526266	73.78%	8.313%
10	7.428	902	908	911	rBV	1971885	2119627	61.91%	6.975%
11	8.145	1025	1030	1033	rBV	1287057	1057034	30.87%	3.478%
12	9.222	1207	1213	1216	rBV	3613475	3423844	100.00%	11.266%
13	9.610	1275	1279	1282	rBV	639746	495323	14.47%	1.630%
14	9.898	1324	1328	1332	rBV2	1264237	1144676	33.43%	3.767%
15	10.322	1397	1400	1403	rVB	53148	40221	1.17%	0.132%
16	10.692	1455	1463	1466	rBV	2007050	2007763	58.64%	6.607%
17	10.792	1477	1480	1488	rVB	58998	58420	1.71%	0.192%
18	11.386	1577	1581	1584	rBV	1352095	1114735	32.56%	3.668%
19	12.975	1846	1851	1854	rBV	2874411	2893748	84.52%	9.522%
20	13.857	1997	2001	2008	rBV2	35673	44133	1.29%	0.145%
21	14.027	2025	2030	2033	rBV	869038	821650	24.00%	2.704%
22	15.121	2209	2216	2220	rBV	30061	35183	1.03%	0.116%
23	15.498	2275	2280	2291	rVB	513085	635066	18.55%	2.090%
24	15.939	2349	2355	2363	rBV	45488	71538	2.09%	0.235%
25	16.445	2435	2441	2450	rBV	46941	82090	2.40%	0.270%
26	17.039	2536	2542	2551	rVB3	32703	70177	2.05%	0.231%
27	17.745	2654	2662	2669	rBV3	30297	71607	2.09%	0.236%
28	18.580	2796	2804	2815	rVB6	20477	64593	1.89%	0.213%

Sum of corrected areas: 30390010

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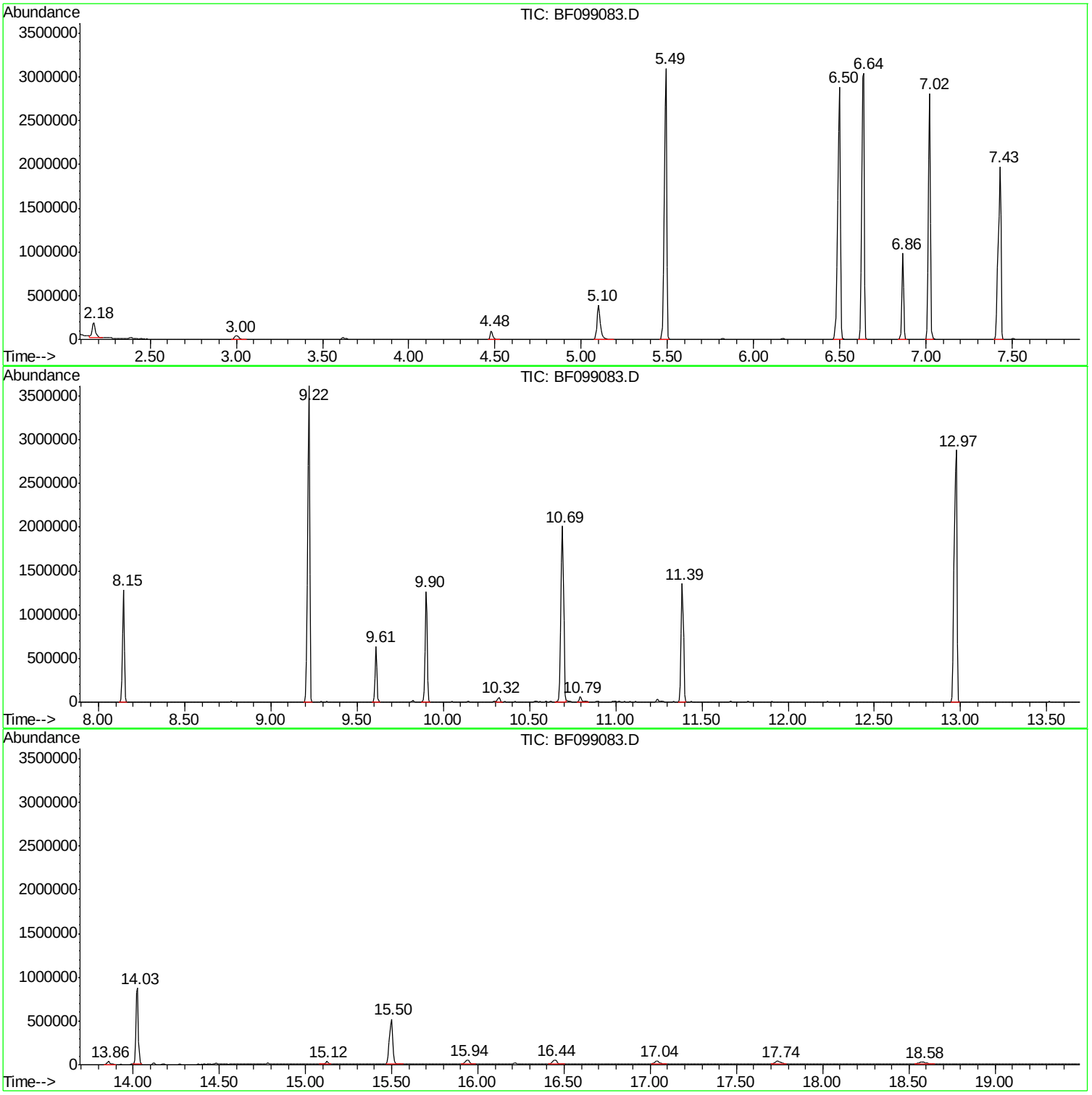
BNA_F
ClientSampleId :
TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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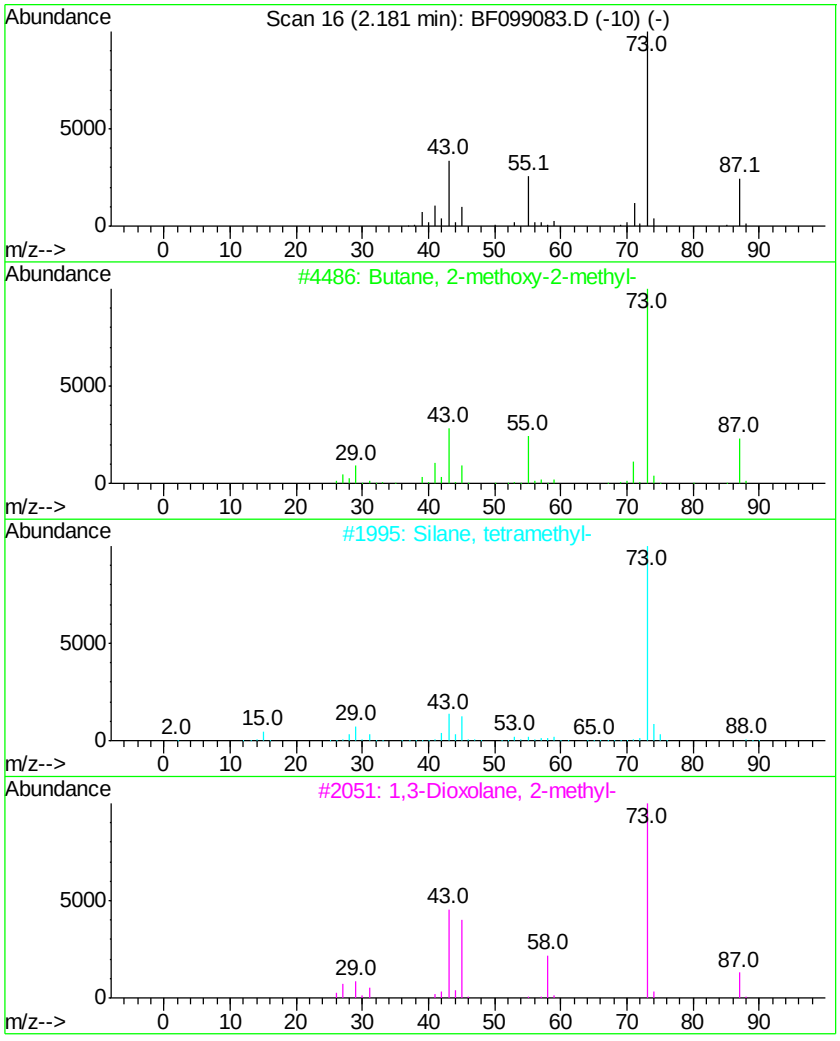
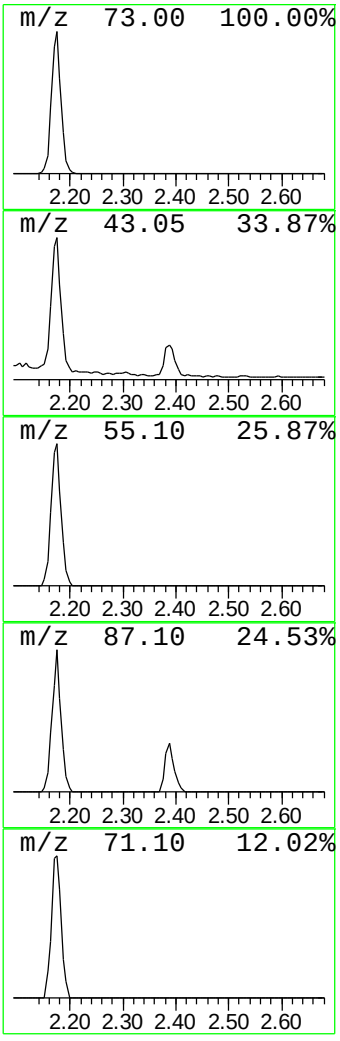
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	6.13 ng	237348	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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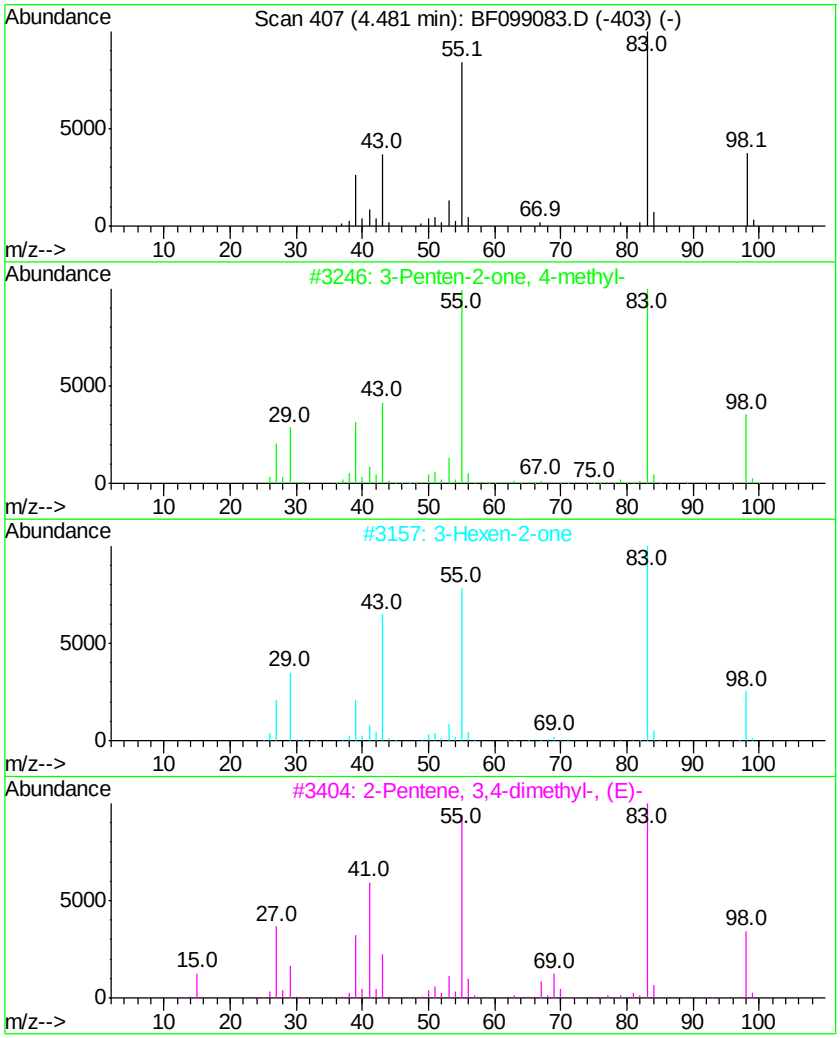
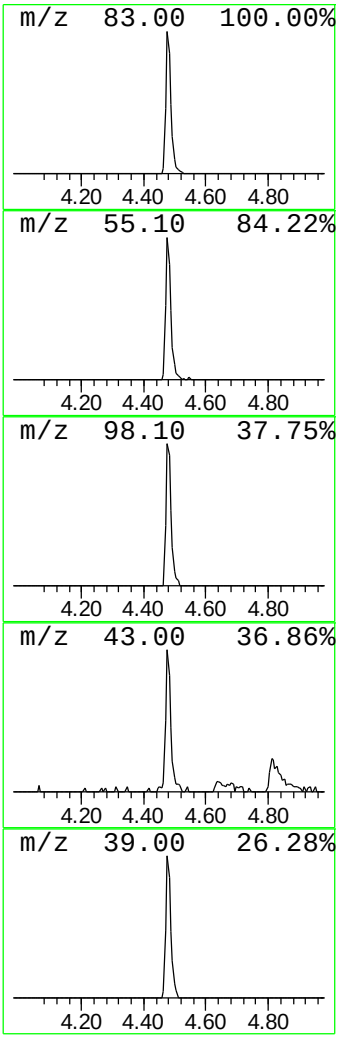
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	2.79 ng	107947	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





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Sample : I5644-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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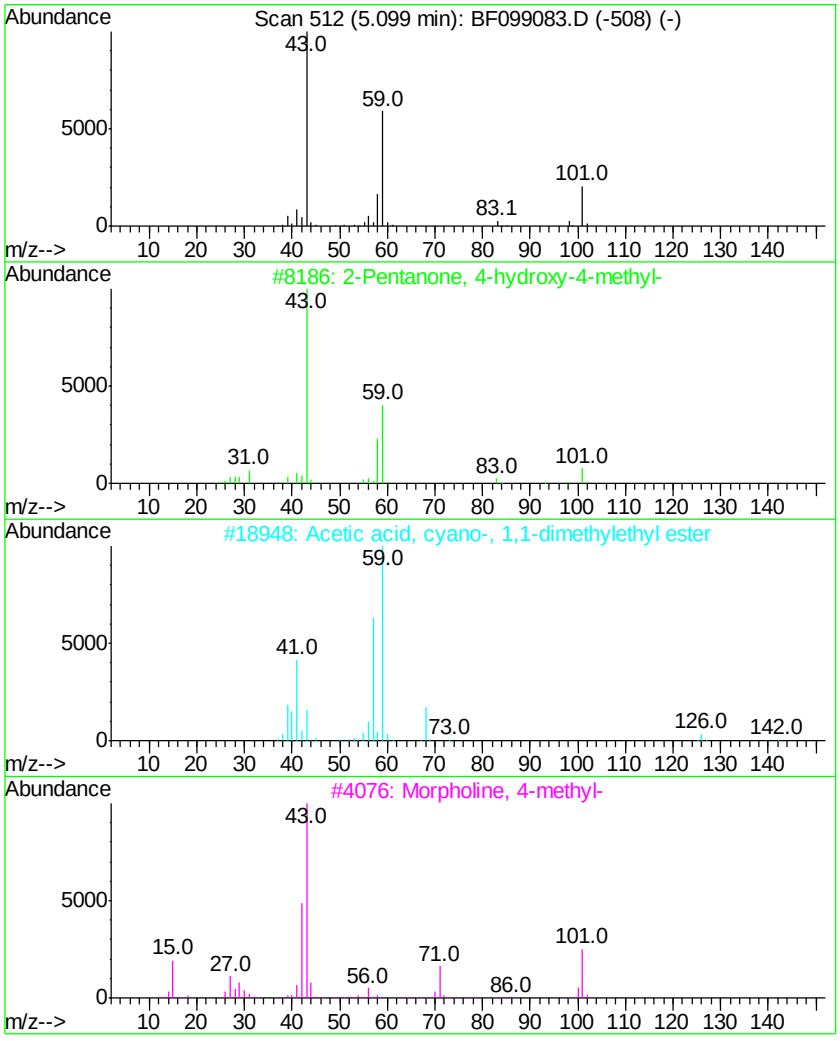
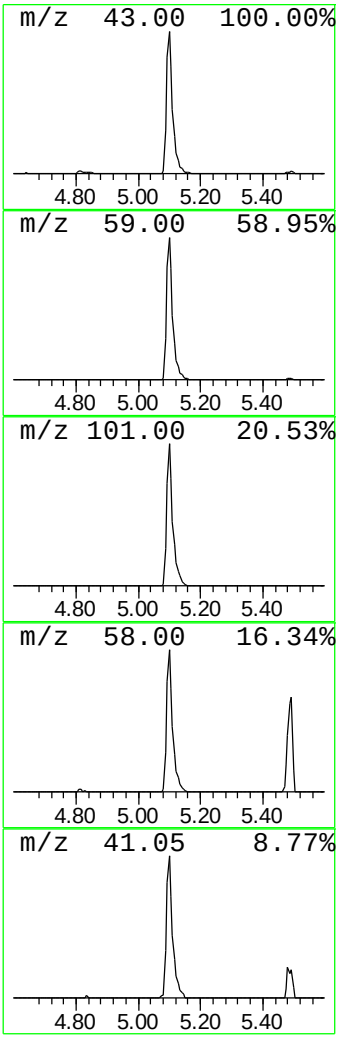
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	14.13 ng	547057	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
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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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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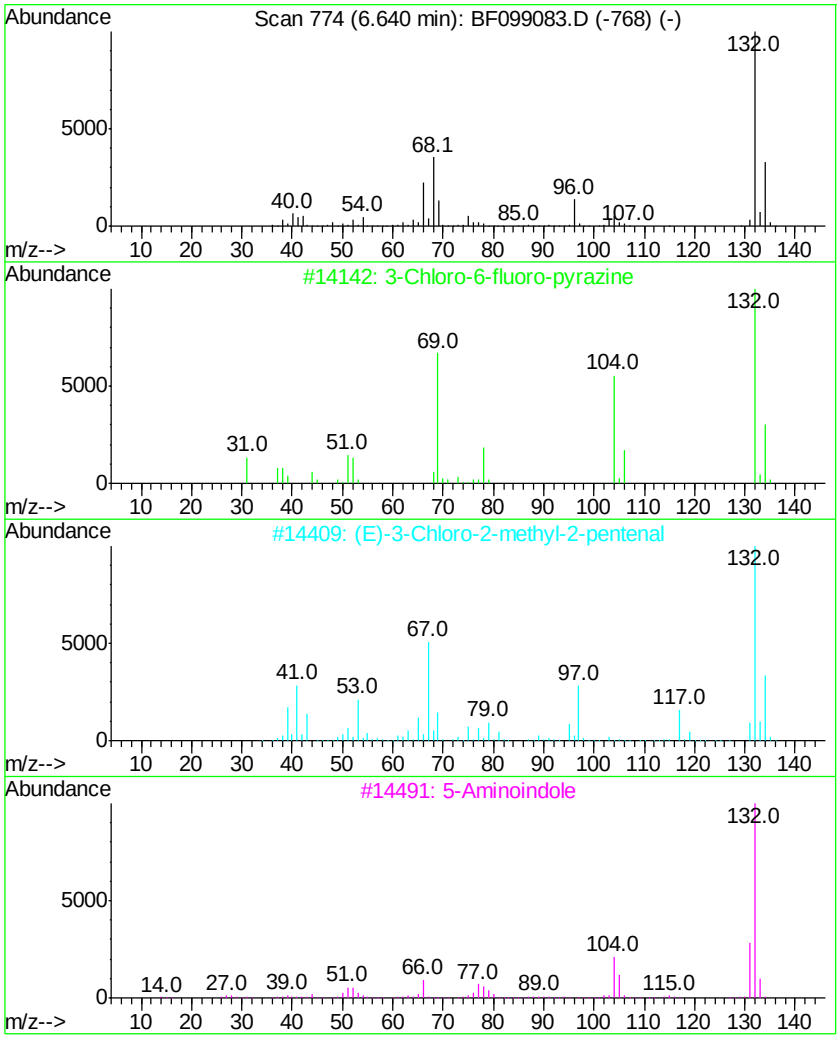
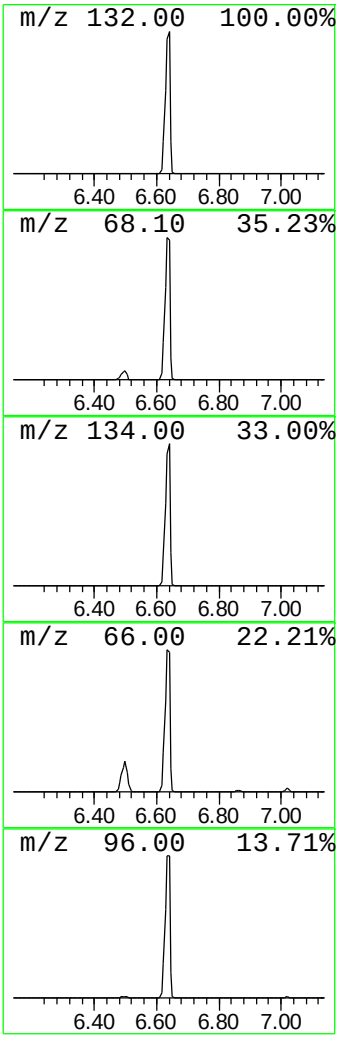
Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	86.25 ng	3338380	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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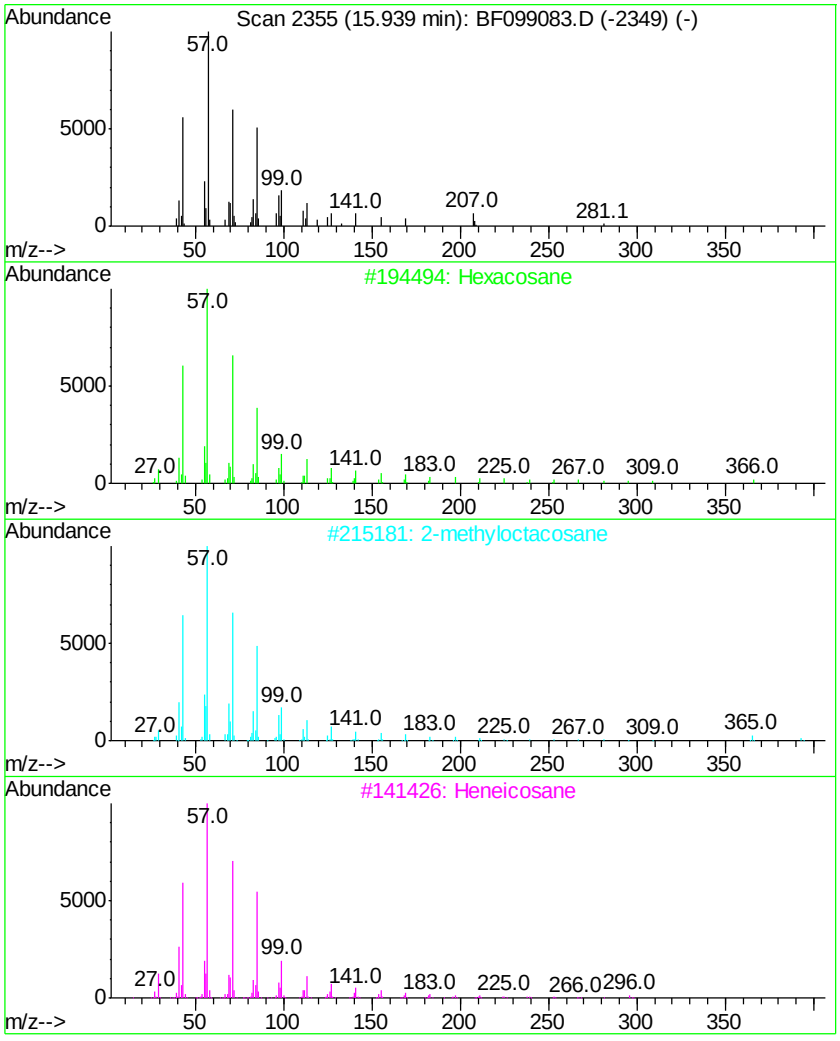
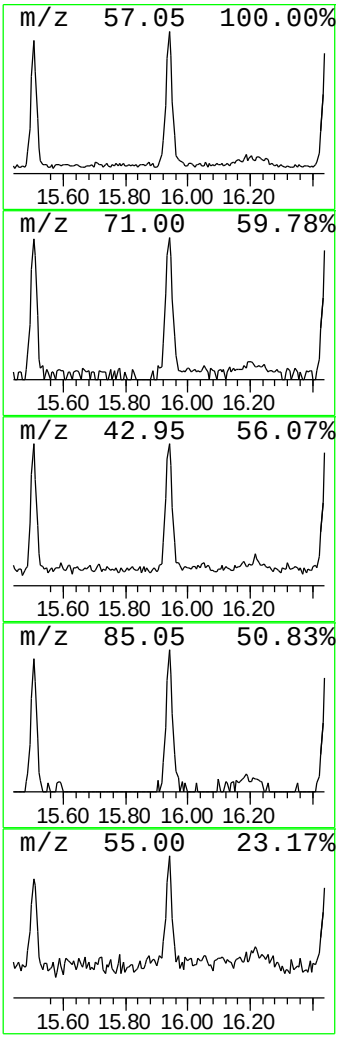
Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.25 ng	71538	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Triacontane	422	C30H62	000638-68-6	86





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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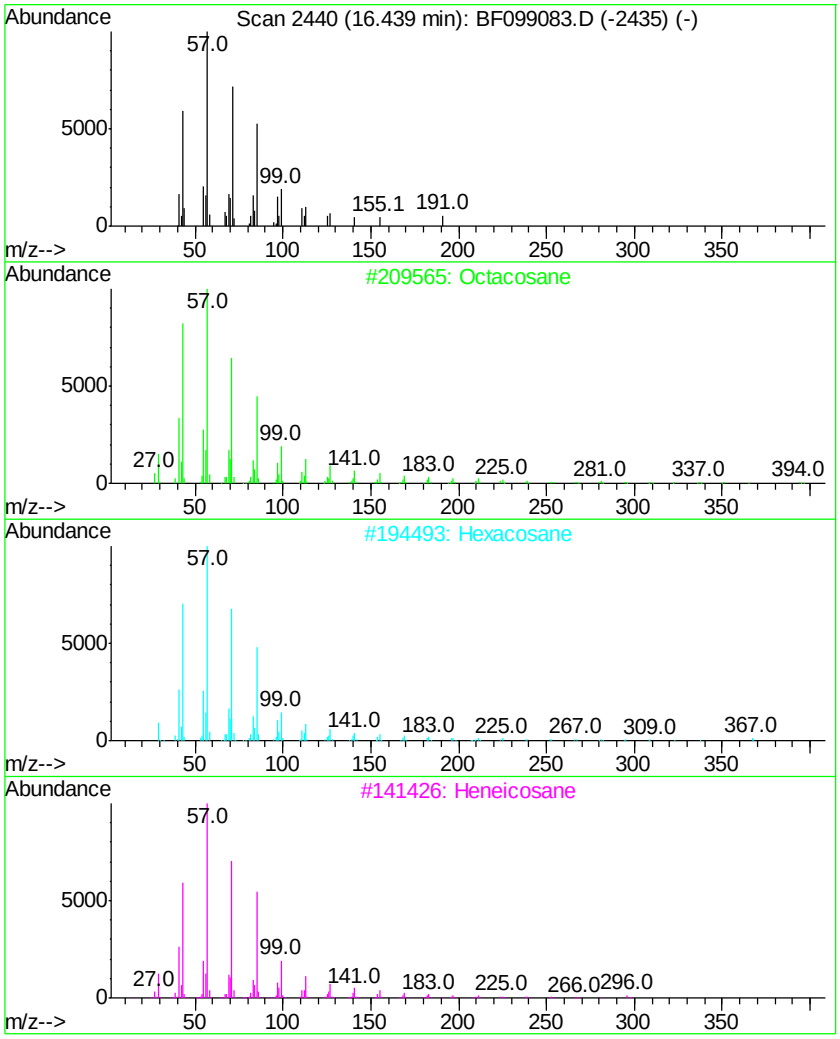
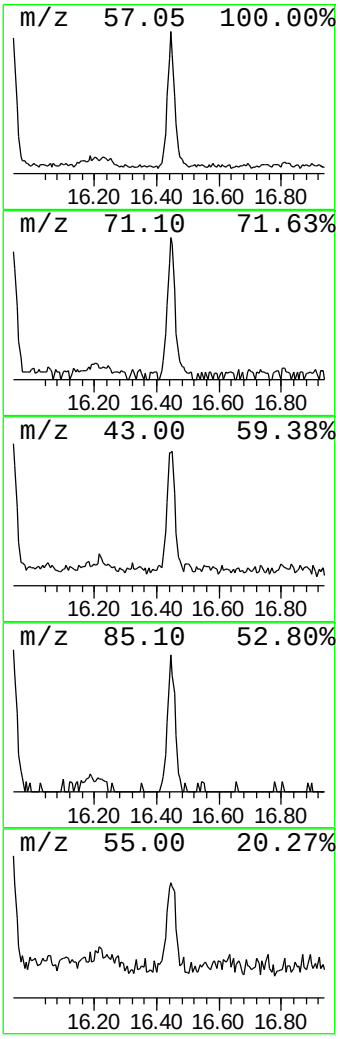
Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.59 ng	82090	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hentriacontane	437	C31H64	000630-04-6	91





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Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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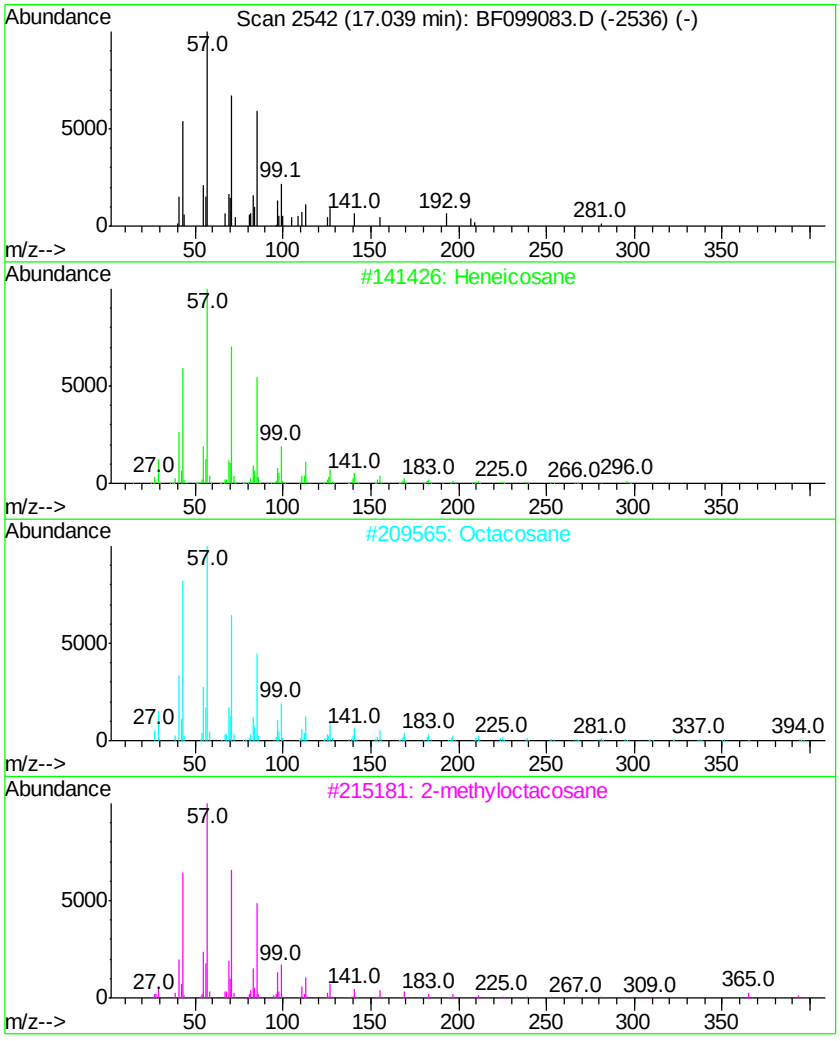
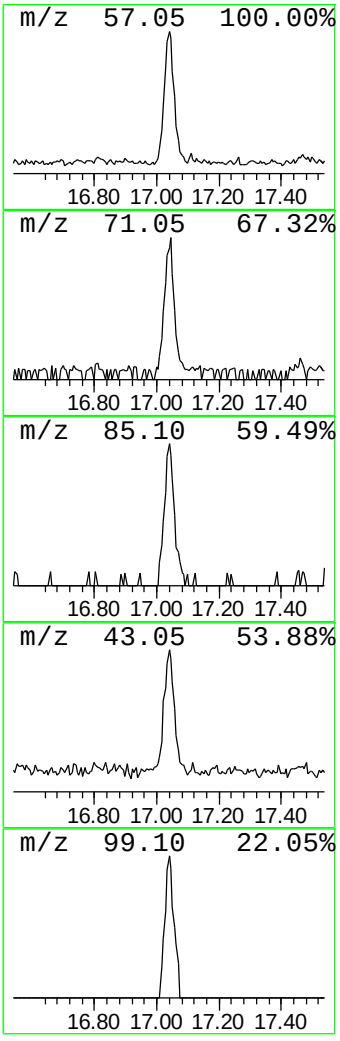
Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	2.21 ng	70177	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Heptadecane	240	C17H36	000629-78-7	90





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Instrument : BNA_F
ClientSampleId : TP-12-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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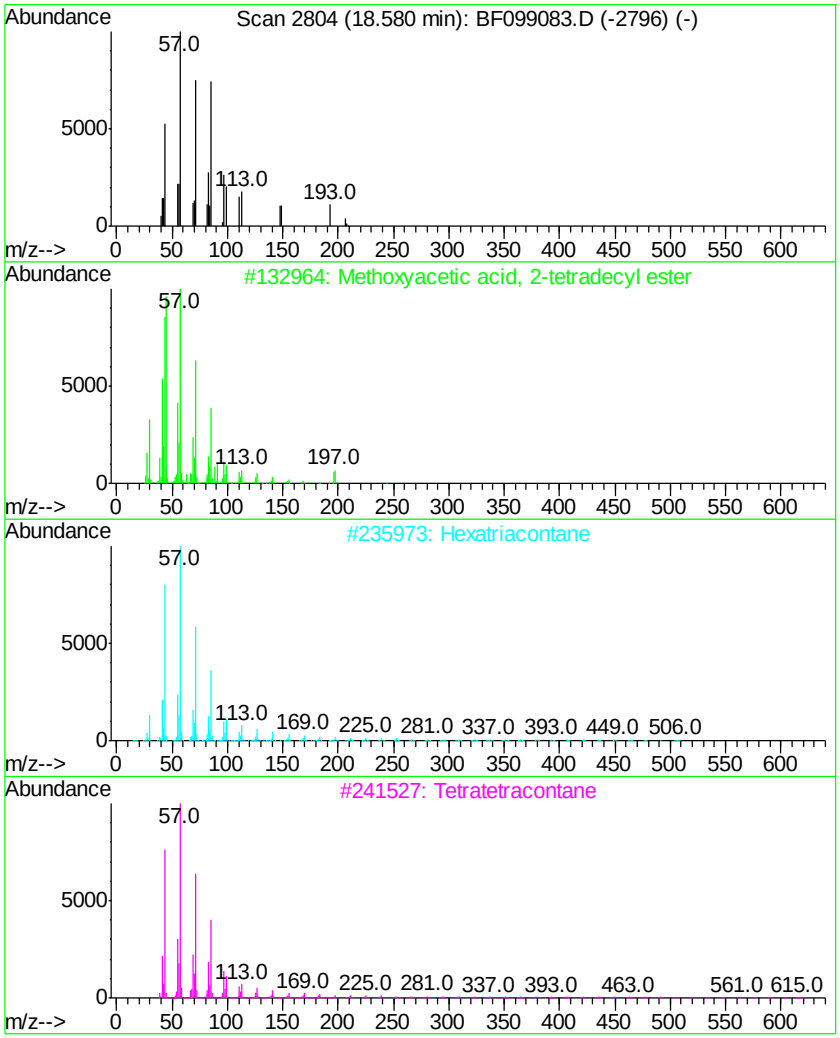
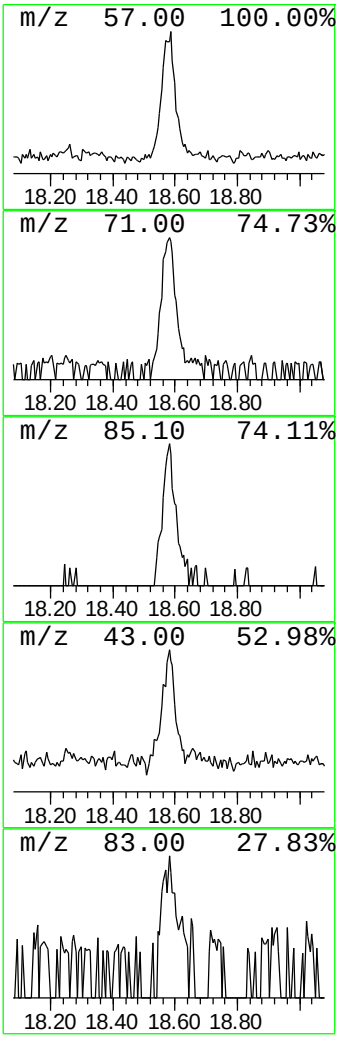
Peak Number 10 Methoxyacetic acid, 2-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.03 ng	64593	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	72
2	Hexatriacontane	507	C36H74	000630-06-8	72
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5	Heptadecane	240	C17H36	000629-78-7	59





Tentatively Identified Compound (LSC) summary

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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...	2.18	6.1	ng	237348	1	6.86	774107	20.0
3-Penten-2-one, 4...	4.48	2.8	ng	107947	1	6.86	774107	20.0
2-Pentanone, 4-hy...	5.10	14.1	ng	547057	1	6.86	774107	20.0
unknown6.64	6.64	86.3	ng	3338380	1	6.86	774107	20.0
Hexacosane	15.94	2.3	ng	71538	6	15.50	635066	20.0
Octacosane	16.44	2.6	ng	82090	6	15.50	635066	20.0
Heneicosane	17.04	2.2	ng	70177	6	15.50	635066	20.0
Methoxyacetic aci...	18.58	2.0	ng	64593	6	15.50	635066	20.0