LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM042617\
Data File : BM009718.D
Acq On : 26 Apr 2017 14:00
Operator : SJ/MA
Sample : I2836-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_M\METHODS\SOM-EPA-BM042517.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.987	657	663	674	rBV	372520	613047	17.82%	1.834%
2	7.157	685	692	699	rBV	289513	450331	13.09%	1.347%
3	7.357	719	726	734	rVB	350114	566571	16.47%	1.695%
4	7.822	797	805	818	rBV	536548	878479	25.54%	2.628%
5	8.522	918	924	934	rBV	401952	683648	19.87%	2.045%
6	8.992	995	1004	1013	rBV	360430	610708	17.75%	1.827%
7	9.710	1119	1126	1136	rBV	297103	493022	14.33%	1.475%
8	10.239	1209	1216	1227	rVB	404253	683723	19.88%	2.046%
9	10.622	1274	1281	1288	rBV	730767	1223120	35.56%	3.659%
10	10.769	1299	1306	1316	rBV	175250	312280	9.08%	0.934%
11	13.880	1829	1835	1839	rBV	805463	1119658	32.55%	3.350%
12	13.921	1839	1842	1849	rVB	177372	251666	7.32%	0.753%
13	14.163	1877	1883	1891	rVB	805785	1210605	35.19%	3.622%
14	14.468	1929	1935	1944	rVB2	1094675	1699934	49.42%	5.086%
15	14.674	1964	1970	1984	rBV	363171	625542	18.18%	1.872%
16	15.298	2071	2076	2082	rVB	59259	69889	2.03%	0.209%
17	15.462	2098	2104	2113	rBV	1140615	1643995	47.79%	4.919%
18	15.592	2119	2126	2132	rBV	398208	572387	16.64%	1.713%
19	15.704	2137	2145	2150	rVV6	28808	53247	1.55%	0.159%
20	16.162	2218	2223	2231	rBV	71485	120838	3.51%	0.362%
21	16.951	2353	2357	2361	rBV	48976	59301	1.72%	0.177%
22	17.221	2397	2403	2409	rBV	1614299	2206736	64.15%	6.602%
23	17.321	2413	2420	2429	rVV	1369700	1919649	55.81%	5.743%
24	17.509	2445	2452	2458	rBV4	37794	55439	1.61%	0.166%
25	17.586	2461	2465	2473	rVB5	22766	41810	1.22%	0.125%
26	18.092	2546	2551	2559	rBV2	149292	221374	6.44%	0.662%
27	19.245	2742	2747	2750	rBV5	25301	40821	1.19%	0.122%
28	19.274	2750	2752	2757	rVB2	58044	75198	2.19%	0.225%
29	19.368	2765	2768	2773	rBV5	59782	87919	2.56%	0.263%
30	19.615	2804	2810	2821	rBV	1958644	2602186	75.65%	7.785%
31	19.721	2824	2828	2837	rVB9	23307	55785	1.62%	0.167%
32	20.109	2890	2894	2896	rBV4	31273	53700	1.56%	0.161%
33	20.274	2919	2922	2927	rBV	40234	43304	1.26%	0.130%
34	21.086	3056	3060	3068	rBV	494048	662030	19.25%	1.981%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_M\METHODS\SOM-EPA-BM042517.M
Title : SVOA CALIBRATION

35	21.397	3108	3113	3124	rBV	2564906	3439909	100.00%	10.292%
36	21.962	3207	3209	3211	rBV2	52955	56113	1.63%	0.168%
37	21.991	3211	3214	3220	rVB4	110517	163306	4.75%	0.489%
38	22.450	3287	3292	3302	rBV	347390	539132	15.67%	1.613%
39	22.574	3310	3313	3318	rVB	125115	160239	4.66%	0.479%
40	22.956	3374	3378	3383	rBV3	301043	435193	12.65%	1.302%
41	23.015	3384	3388	3394	rVB5	177206	286122	8.32%	0.856%
42	23.568	3474	3482	3489	rBV	1387376	2701036	78.52%	8.081%
43	23.715	3500	3507	3515	rVB	1575116	3089344	89.81%	9.243%
44	24.209	3587	3591	3599	rVB	200249	365914	10.64%	1.095%
45	24.303	3605	3607	3615	rVB8	105511	179271	5.21%	0.536%

Sum of corrected areas: 33423521

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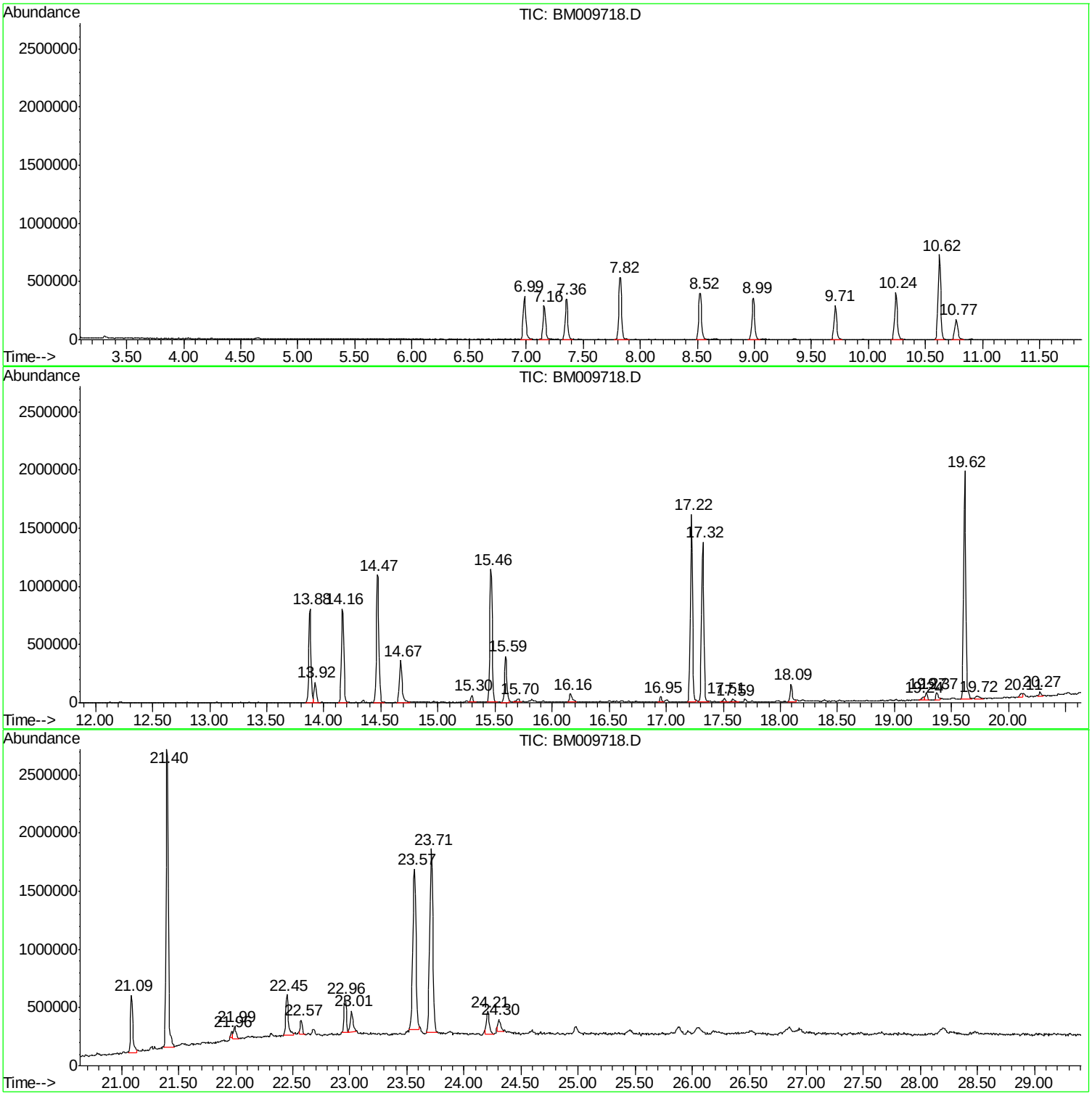
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

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Acq On : 26 Apr 2017 14:00
Operator : SJ/MA
Sample : I2836-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

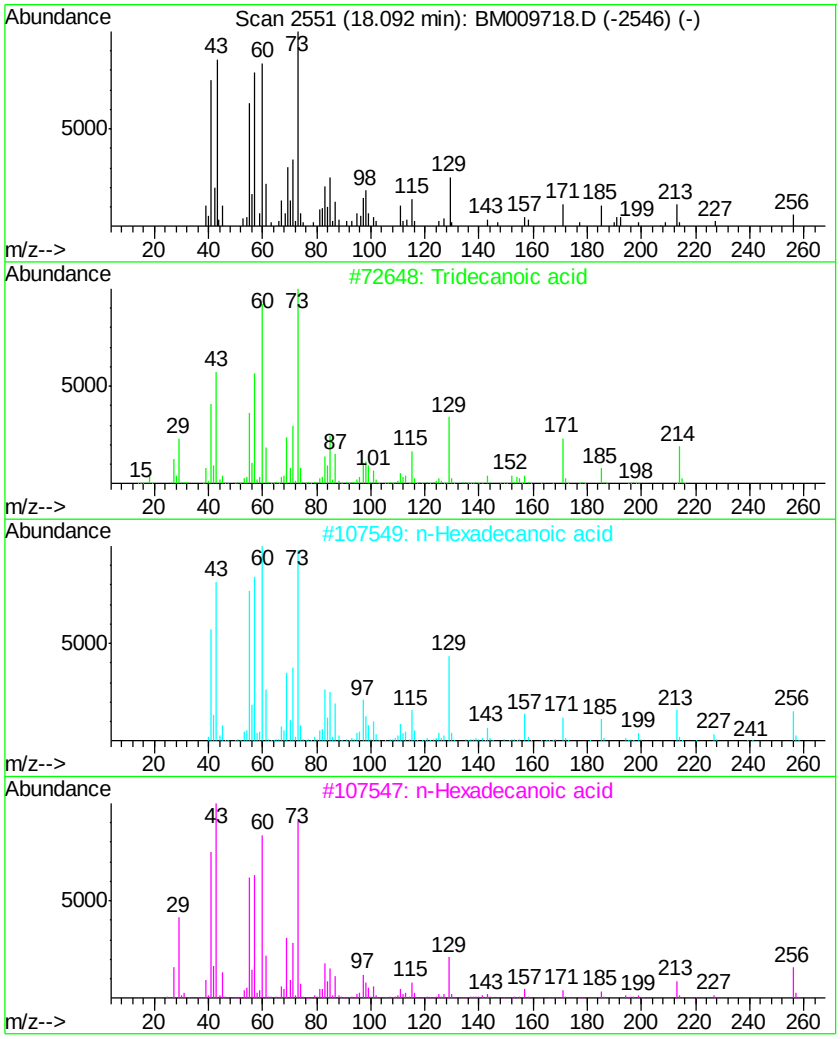
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

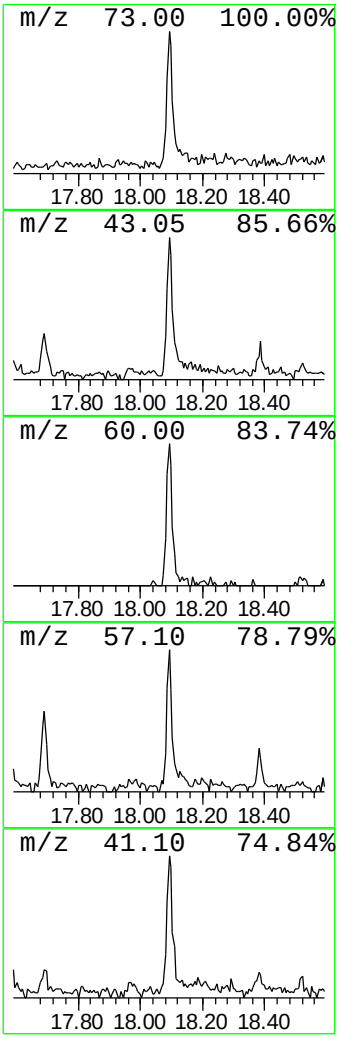
****

Peak Number 1 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	2.01 ng/ul	221374	Phenanthrene-d10	17.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	81
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Acq On : 26 Apr 2017 14:00
Operator : SJ/MA
Sample : I2836-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

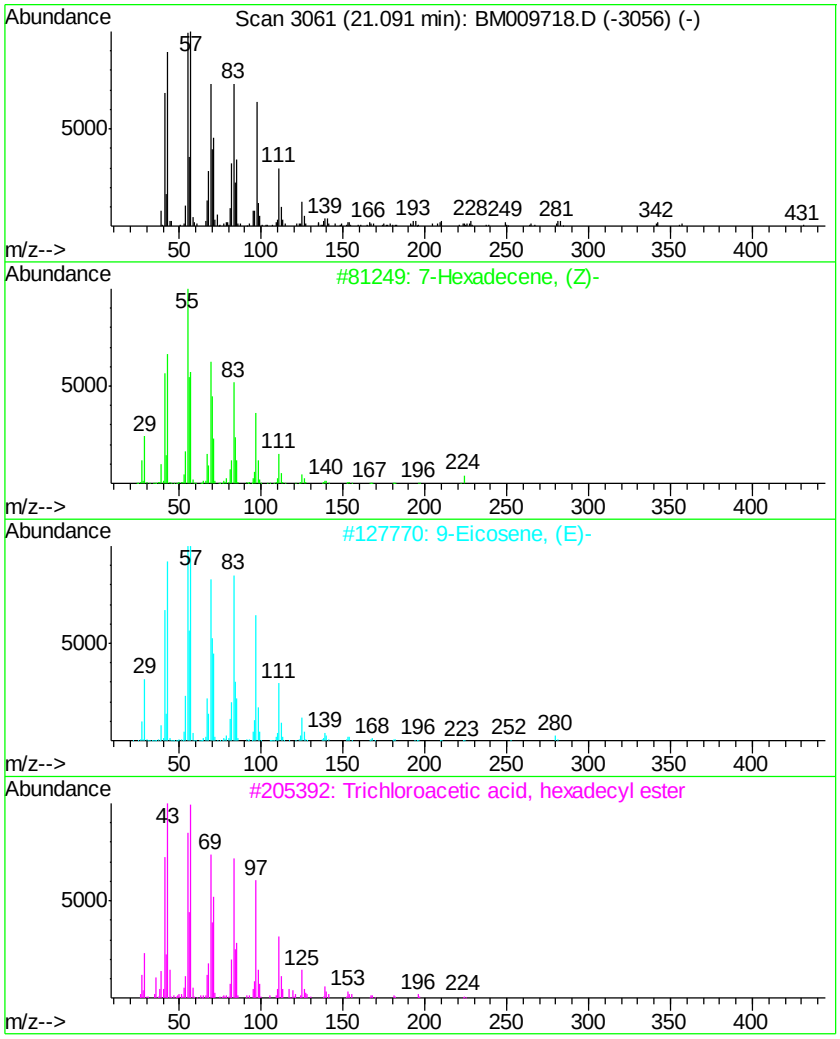
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

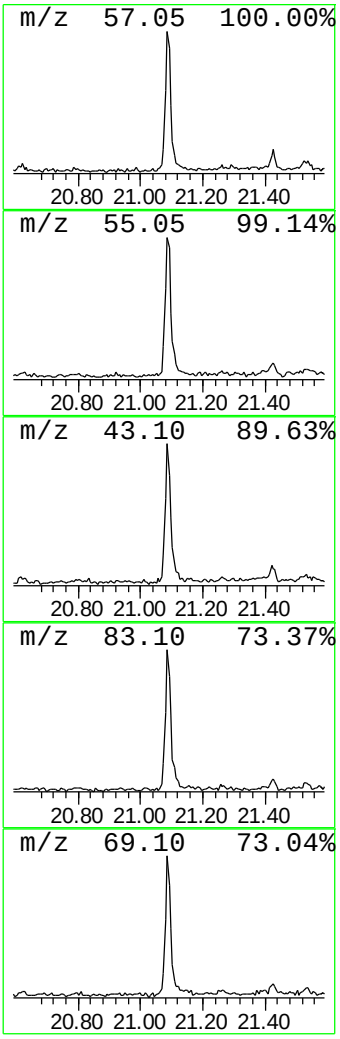
****

Peak Number 2 (DEL) Alkane: Cyclic21.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.09	3.85 ng/ul	662030	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	93
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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Sample : I2836-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CEM-BF002-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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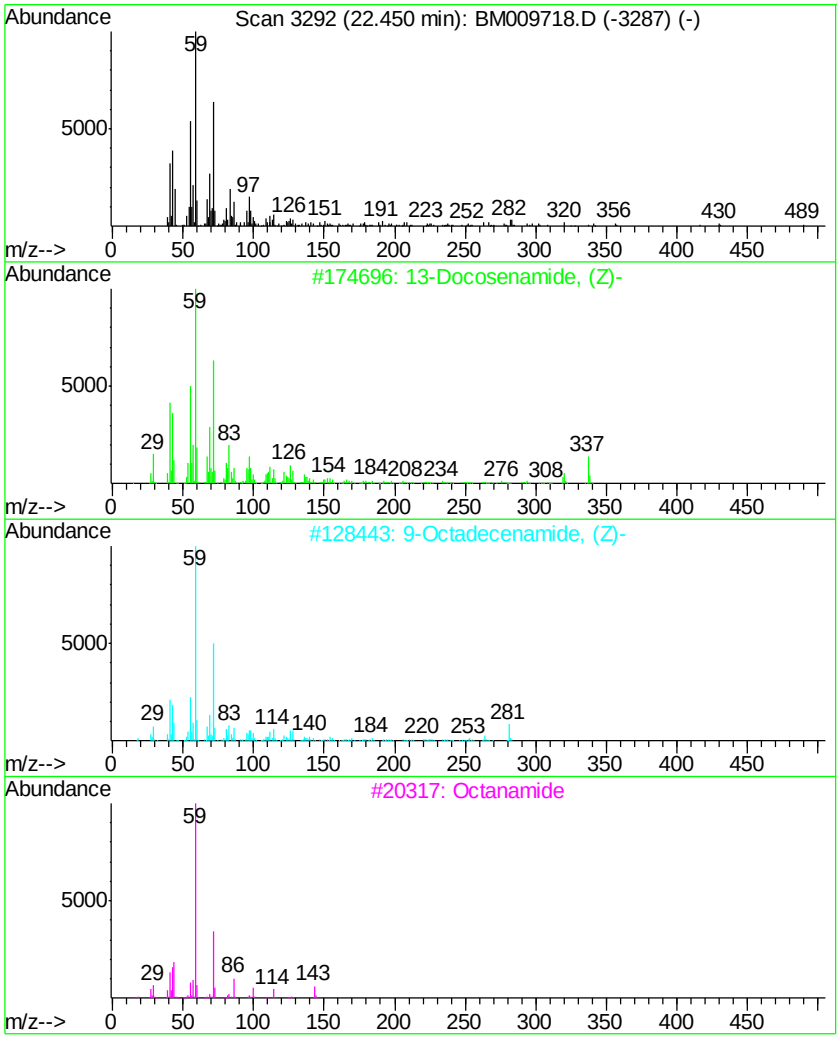
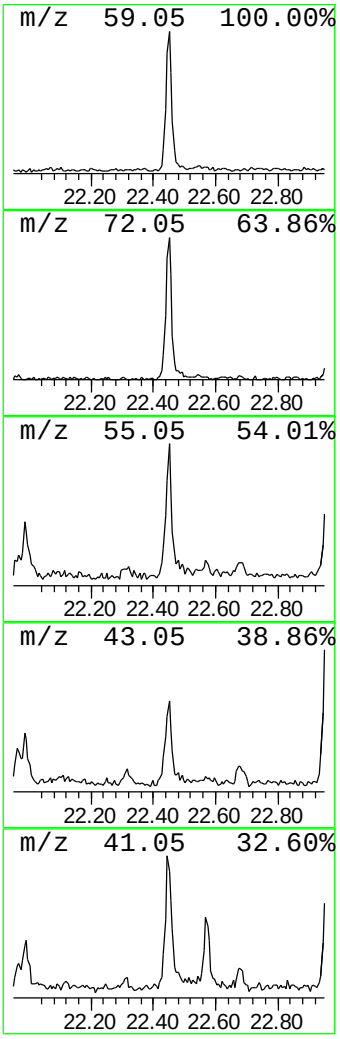
****
Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	3.13 ng/ul	539132	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Octadecanamide	283	C18H37NO	000124-26-5	52





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Instrument :
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ClientSampleId :
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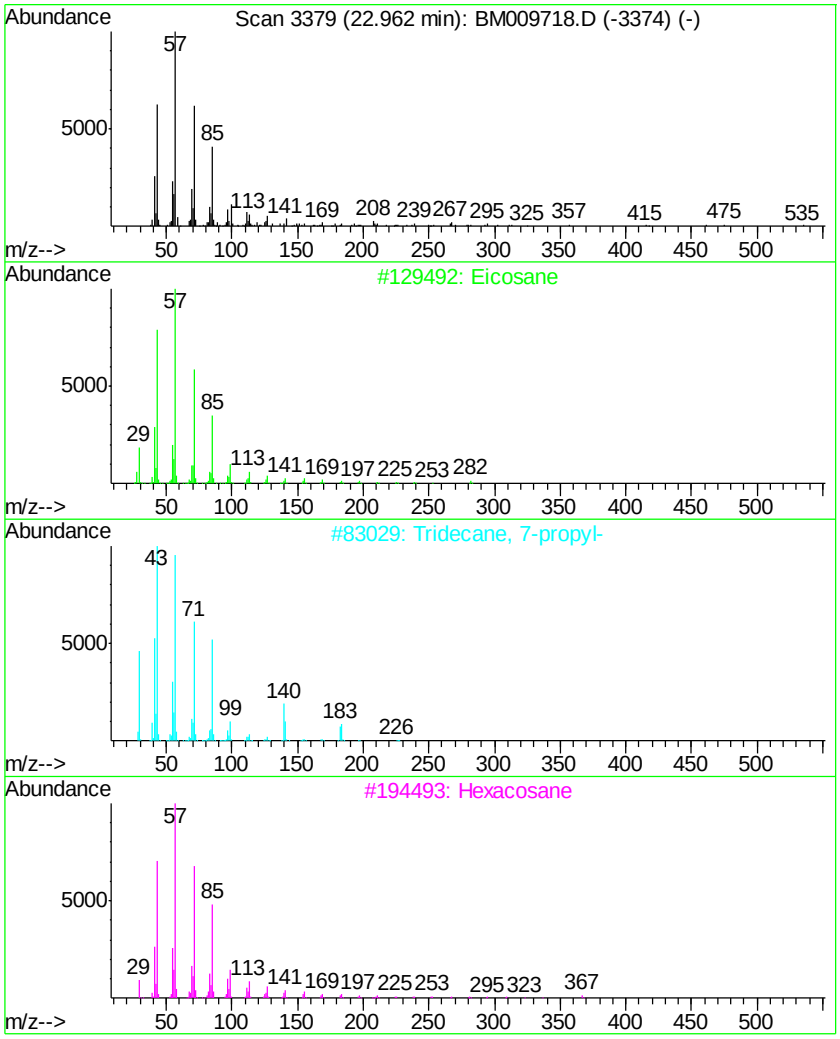
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

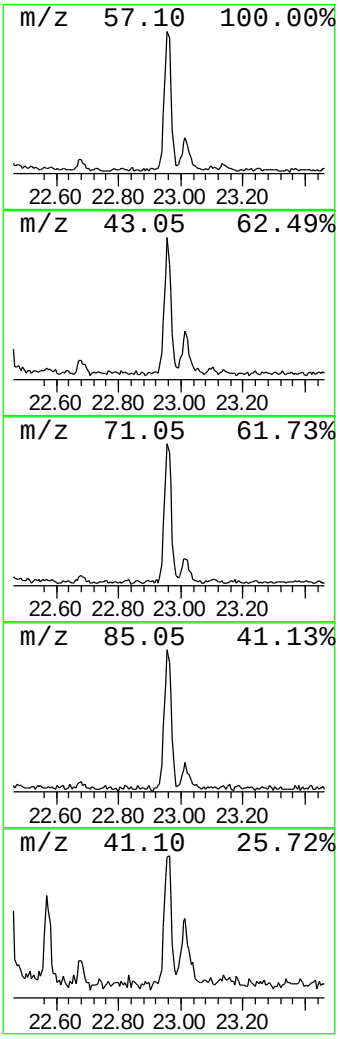
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	2.82 ng/ul	435193	Perylene-d12	23.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Tetracosane	338	C24H50	000646-31-1	87





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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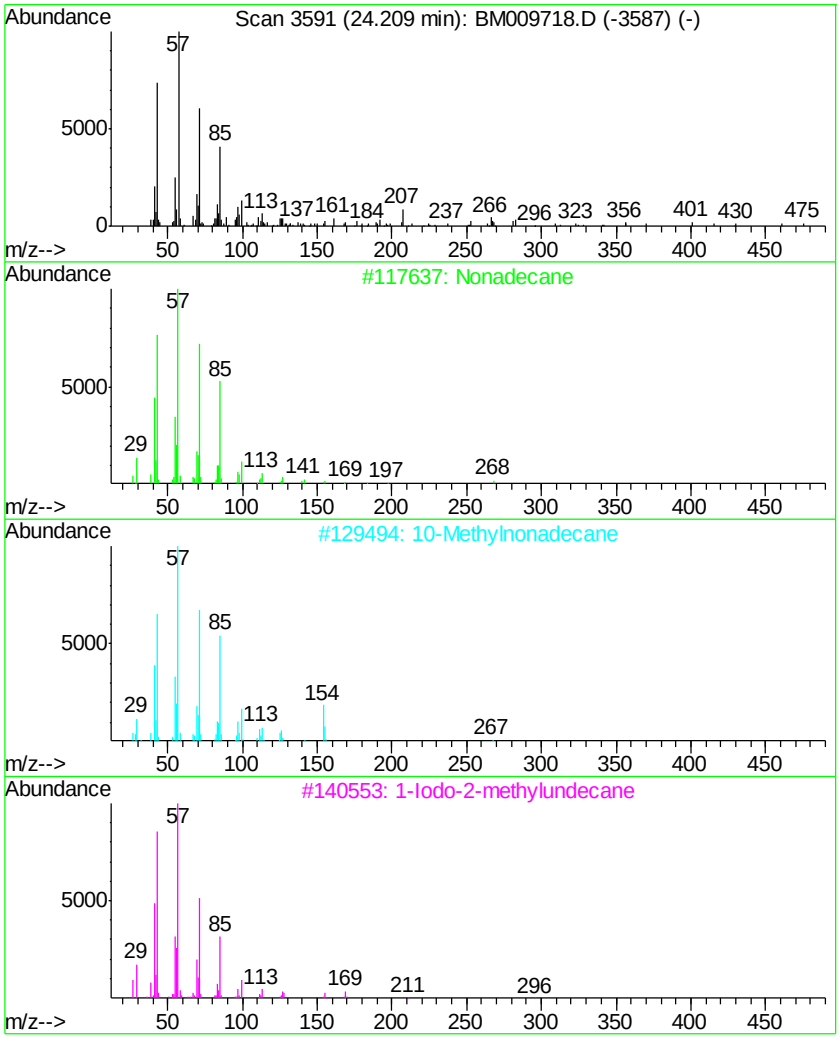
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

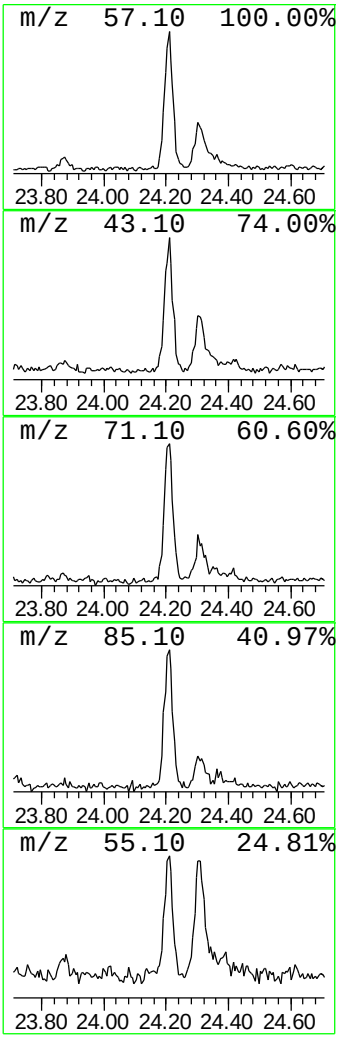
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.21	2.37 ng/ul	365914	Perylene-d12	23.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	10-Methylnonadecane	282	C20H42	056862-62-5	87
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Hexacosane	366	C26H54	000630-01-3	80





Tentatively Identified Compound (LSC) summary

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Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Tridecanoic acid	18.09	2.0	ng/ul	221374	4	17.22	2206740	20.0
(DEL) Alkane: Cyc...	21.09	3.9	ng/ul	662030	5	21.40	3439910	20.0
13-Docosenamide, ...	22.45	3.1	ng/ul	539132	5	21.40	3439910	20.0
(DEL) Alkane: Str...	22.96	2.8	ng/ul	435193	6	23.71	3089340	20.0
(DEL) Alkane: Str...	24.21	2.4	ng/ul	365914	6	23.71	3089340	20.0