LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM062216\
Data File : BM005931.D
Acq On : 23 Jun 2016 15:32
Operator : UM/SJ
Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

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\SOM02.2-EPA-BM062216.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	3.440	142	145	155	rBV	180139	257531	2.02%	0.139%
2	6.834	714	722	738	rBV	3059173	5142274	40.29%	2.784%
3	7.004	740	751	762	rBV	2394652	3819967	29.93%	2.068%
4	7.198	776	784	793	rBV	3110211	5032396	39.43%	2.724%
5	7.663	854	863	871	rBV	2766292	4497757	35.24%	2.435%
6	8.369	972	983	994	rBV	3710293	6385860	50.04%	3.457%
7	8.816	1050	1059	1072	rBV	2956852	5123331	40.14%	2.773%
8	9.534	1172	1181	1196	rBV	2572617	4327418	33.91%	2.342%
9	10.063	1262	1271	1288	rBV	3593931	6330517	49.60%	3.427%
10	10.445	1328	1336	1348	rVB	3776983	6673633	52.29%	3.613%
11	10.581	1350	1359	1377	rBV	3257157	6100662	47.80%	3.302%
12	12.039	1600	1607	1617	rVB2	73880	133469	1.05%	0.072%
13	13.727	1887	1894	1898	rBV	5694979	8473763	66.40%	4.587%
14	13.774	1898	1902	1911	rVB	1967577	2866462	22.46%	1.552%
15	14.004	1931	1941	1952	rBV	6314564	10214816	80.04%	5.529%
16	14.221	1973	1978	1986	rBV	140270	221149	1.73%	0.120%
17	14.310	1986	1993	2004	rVB2	4786003	8123184	63.65%	4.397%
18	14.510	2019	2027	2045	rBV	2944450	4608569	36.11%	2.495%
19	15.180	2136	2141	2147	rBV	240213	319782	2.51%	0.173%
20	15.310	2155	2163	2170	rBV	7589568	11663108	91.39%	6.313%
21	15.427	2176	2183	2191	rBV	2647975	3795477	29.74%	2.055%
22	15.545	2198	2203	2207	rBV2	131125	229330	1.80%	0.124%
23	16.039	2282	2287	2304	rBV	280777	605102	4.74%	0.328%
24	16.833	2417	2422	2427	rBV2	230355	350618	2.75%	0.190%
25	17.062	2454	2461	2470	rBV2	5678747	8768353	68.71%	4.746%
26	17.162	2470	2478	2489	rVB2	7313021	11697136	91.65%	6.332%
27	17.962	2609	2614	2624	rBV2	445773	691757	5.42%	0.374%
28	19.086	2800	2805	2810	rBV	132347	203930	1.60%	0.110%
29	19.251	2828	2833	2842	rBV2	150479	239527	1.88%	0.130%
30	19.339	2844	2848	2853	rVB	103059	141686	1.11%	0.077%
31	19.456	2862	2868	2877	rVB2	8064170	12689924	99.43%	6.869%
32	20.974	3121	3126	3135	rBV	1102149	1444570	11.32%	0.782%
33	21.250	3167	3173	3186	rBV	6731006	9278898	72.71%	5.023%
34	21.862	3272	3277	3279	rBV2	221524	397619	3.12%	0.215%

LSC Area Percent Report

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Data File : BM005931.D
Acq On : 23 Jun 2016 15:32
Operator : UM/SJ
Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

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\SOM02.2-EPA-BM062216.M
Title : SVOA CALIBRATION

35	22.015	3298	3303	3308	rBV	499756	656629	5.15%	0.355%
36	22.309	3350	3353	3358	rVB	125450	171822	1.35%	0.093%
37	22.815	3433	3439	3443	rBV	1041101	1643108	12.87%	0.889%
38	23.333	3519	3527	3541	rBV2	6039801	12762271	100.00%	6.908%
39	23.474	3543	3551	3570	rVB2	4593698	9212516	72.19%	4.987%
40	24.015	3637	3643	3650	rBV	508929	1017250	7.97%	0.551%
41	24.097	3651	3657	3665	rVB	336146	701069	5.49%	0.379%
42	24.756	3762	3769	3781	rBV	304792	752180	5.89%	0.407%
43	25.615	3908	3915	3928	rVB2	231404	691620	5.42%	0.374%
44	26.627	4081	4087	4105	rVB3	203943	702336	5.50%	0.380%
45	27.044	4148	4158	4175	rVB2	864576	2930262	22.96%	1.586%
46	27.232	4181	4190	4202	rBV2	422675	1333185	10.45%	0.722%
47	27.821	4284	4290	4310	rVB4	378101	1311899	10.28%	0.710%

Sum of corrected areas: 184735722

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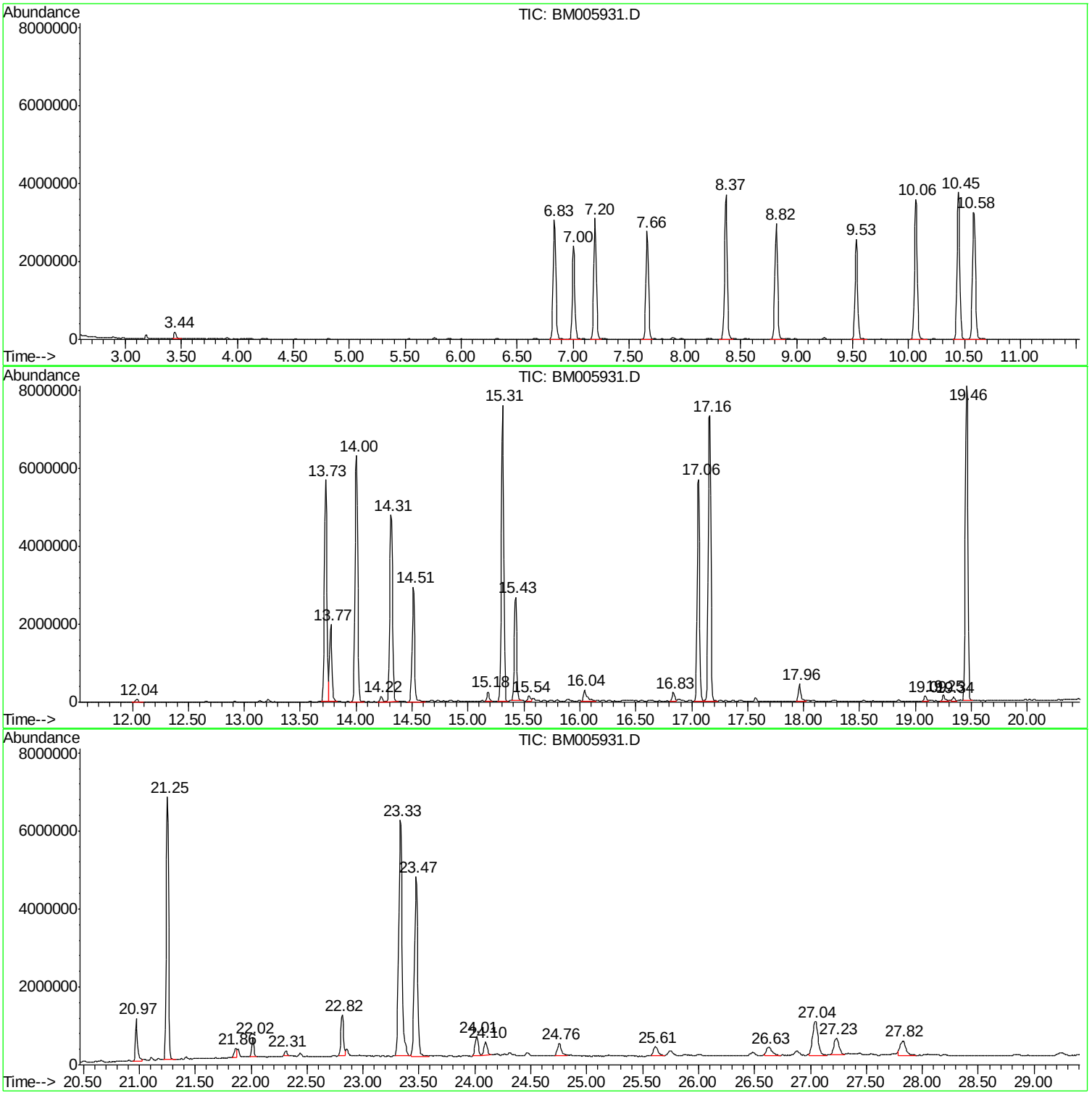
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM062216\
Data File : BM005931.D
Acq On : 23 Jun 2016 15:32
Operator : UM/SJ
Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

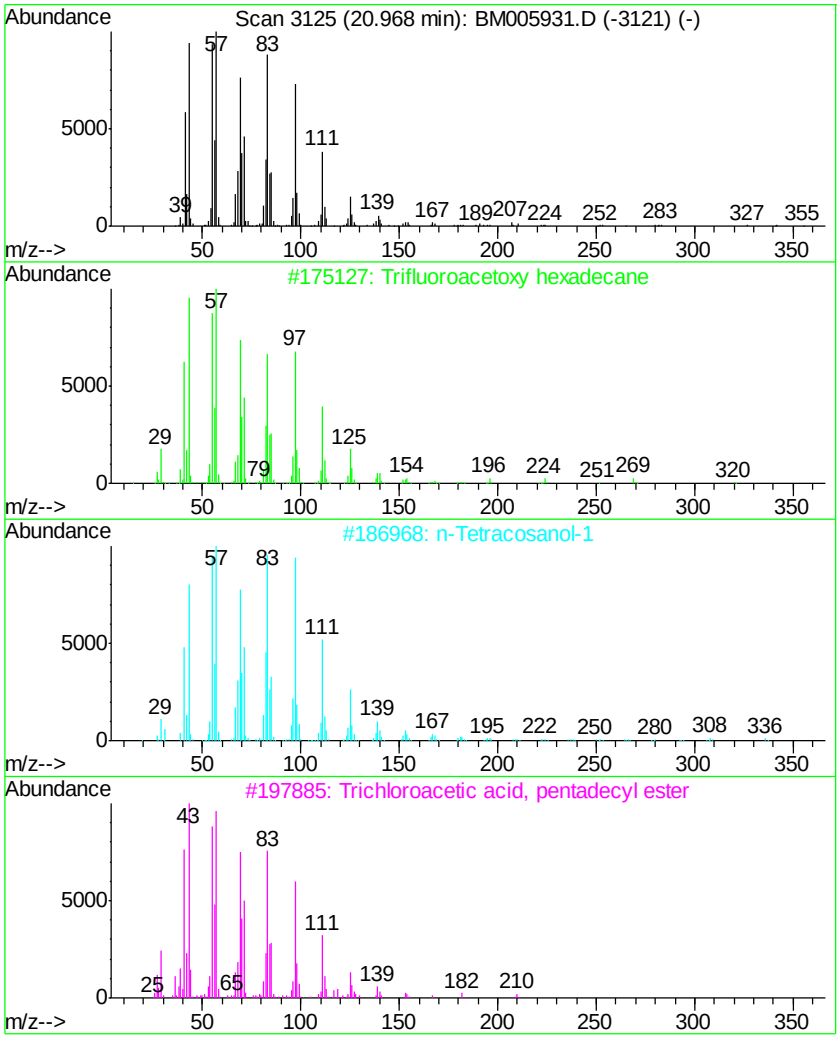
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

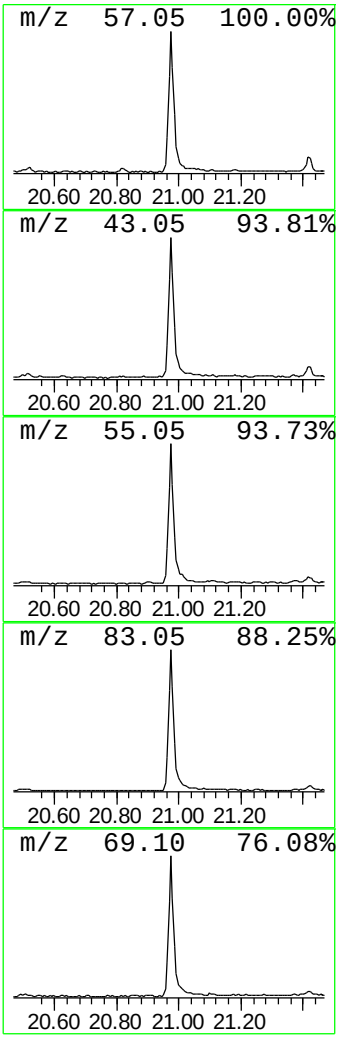
****

Peak Number 1 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	3.11 ng/ul	1444570	Chrysene-d12	21.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Data Path : Z:\HPCHEM1\BNA M\DATA\BM062216\
Data File : BM005931.D
Acq On : 23 Jun 2016 15:32
Operator : UM/SJ
Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

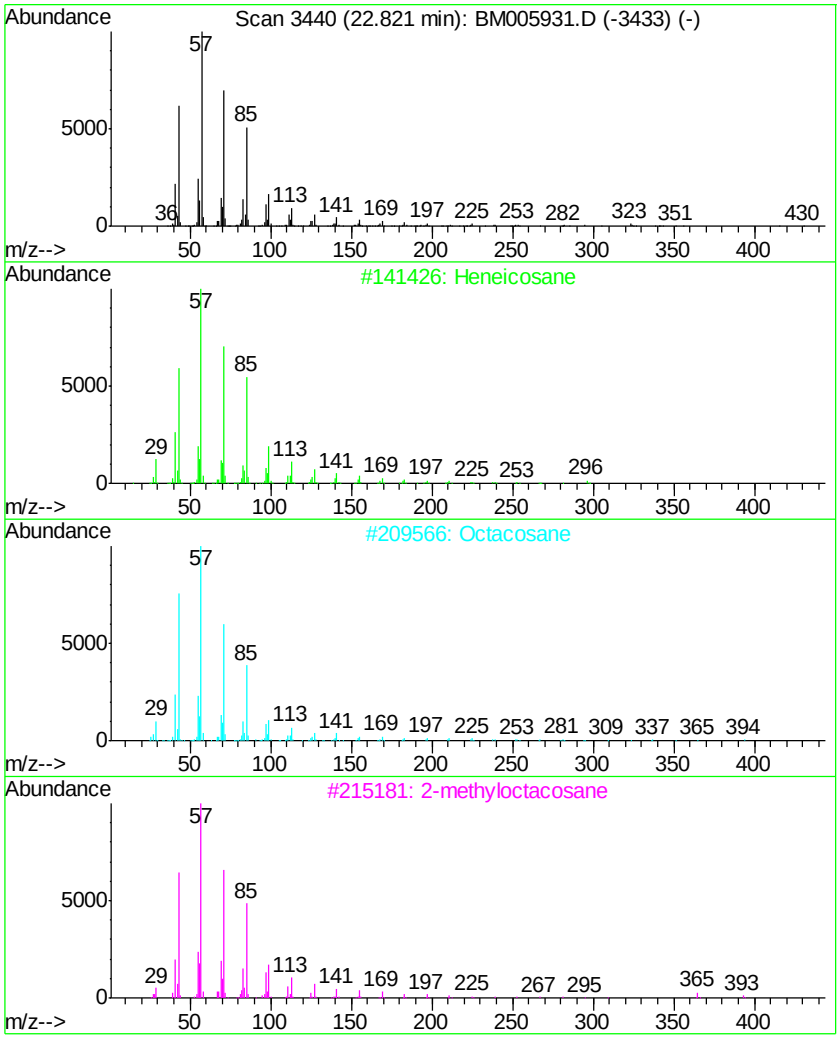
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

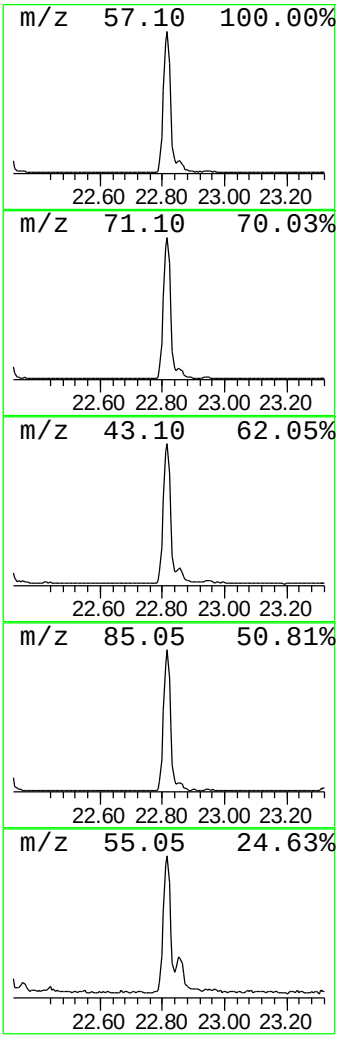
****

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.82	3.57 ng/ul	1643110	Perylene-d12	23.47

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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexadecane	226	C16H34	000544-76-3	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM062216\
Data File : BM005931.D
Acq On : 23 Jun 2016 15:32
Operator : UM/SJ
Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

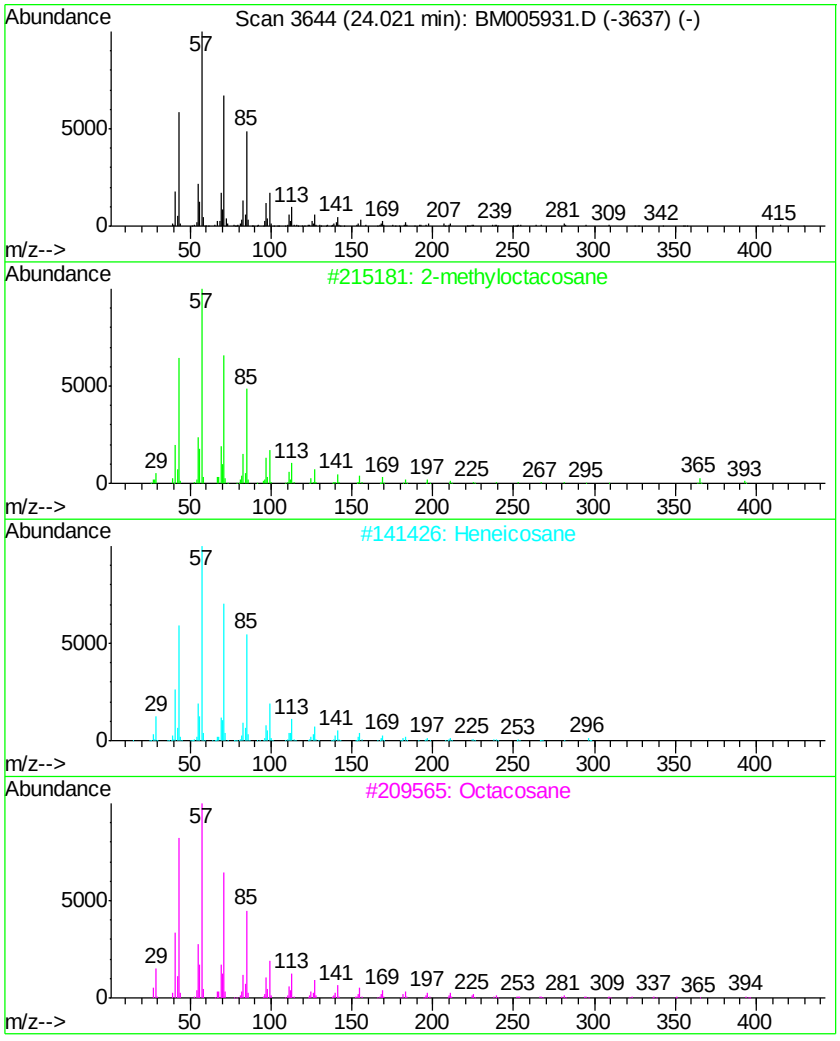
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

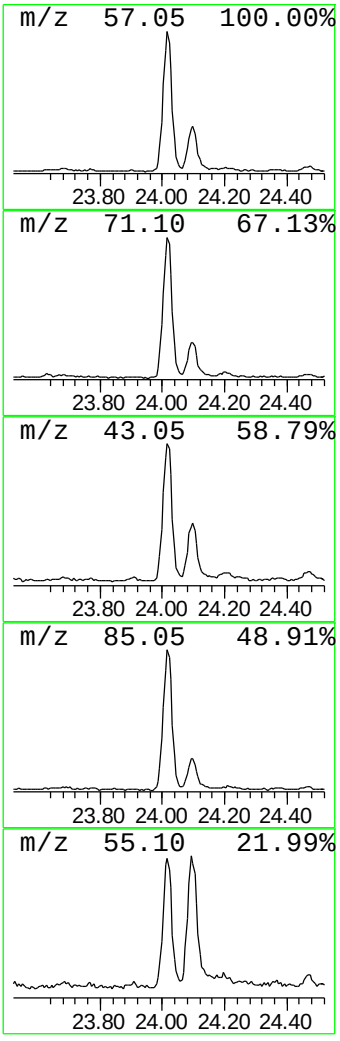
****

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.02	2.21 ng/ul	1017250	Perylene-d12	23.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Sample : H3612-17
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

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

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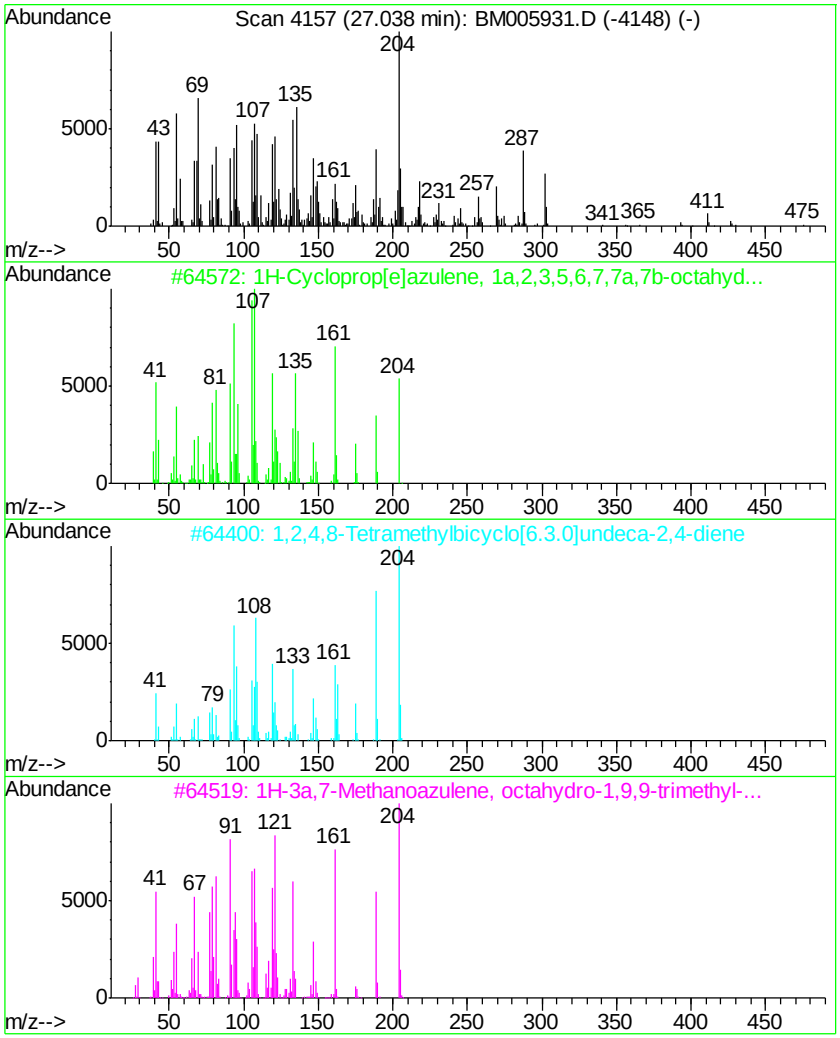
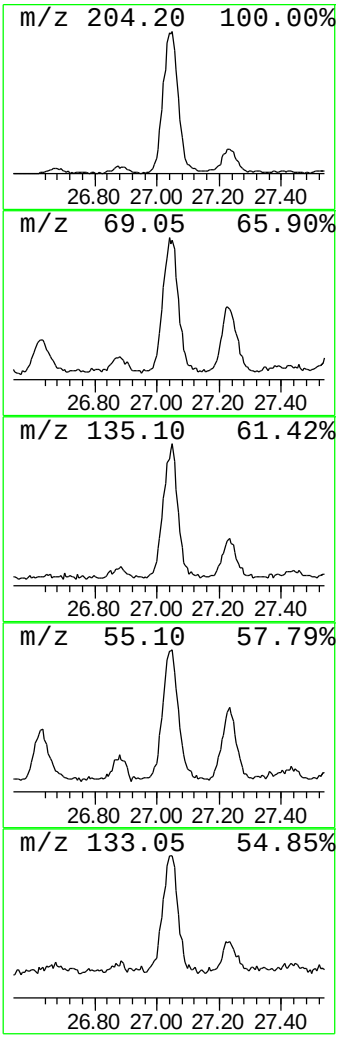
Peak Number 4 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.04	6.36 ng/ul	2930260	Perylene-d12	23.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	50
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
3	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	43
4	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	43
5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	43





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

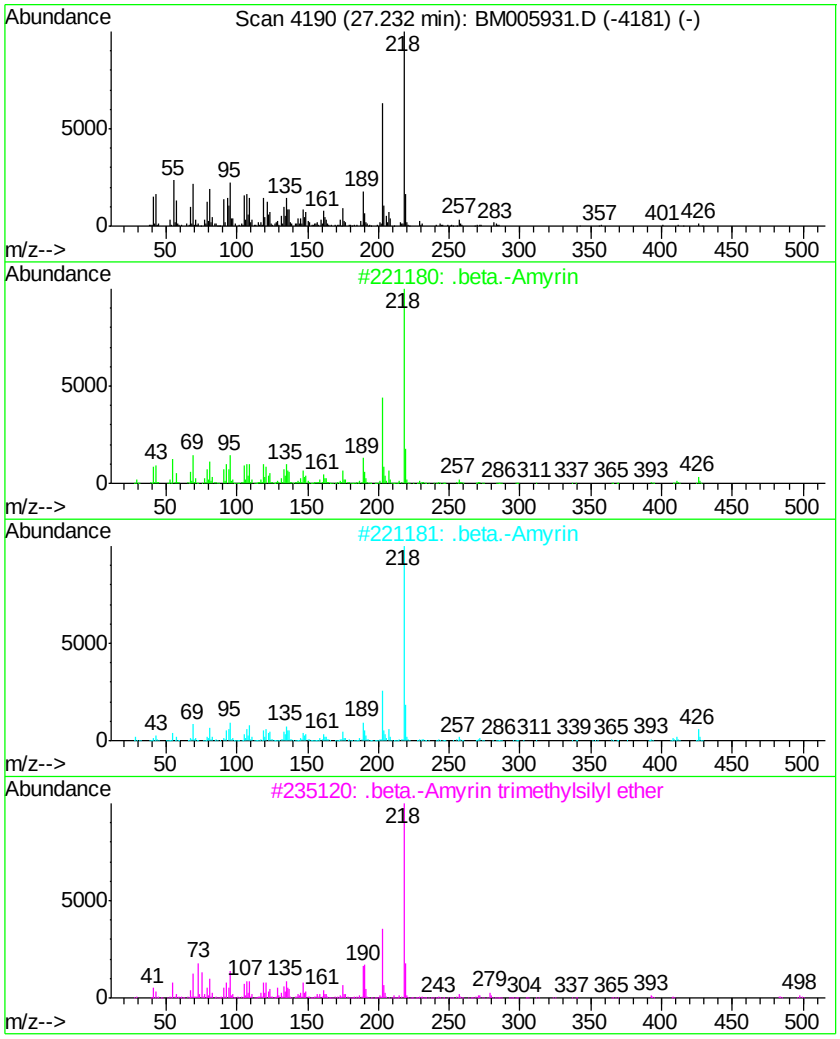
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

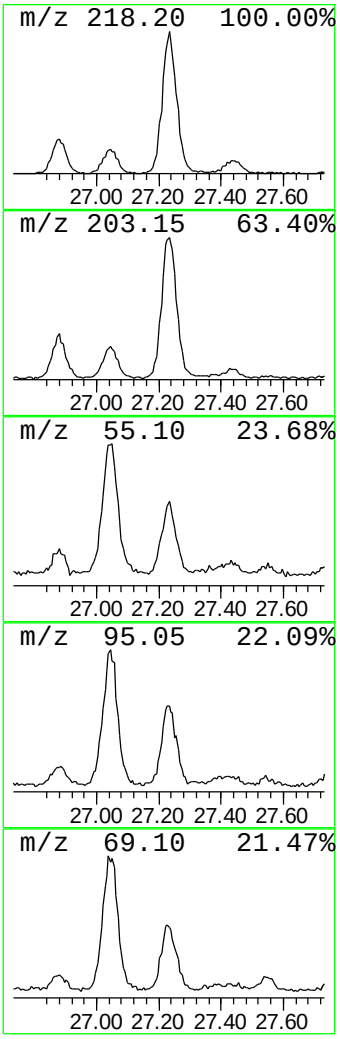
****

Peak Number 5 .beta.-Amyrin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.23	2.89 ng/ul	1333190	Perylene-d12	23.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	91
2	.beta.-Amyrin	426	C30H50O	000559-70-6	80
3	.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	72
4	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	70
5	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	68





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ClientSampleId : D9Z35

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM062216.M
Quant Title : SVOA CALIBRATION

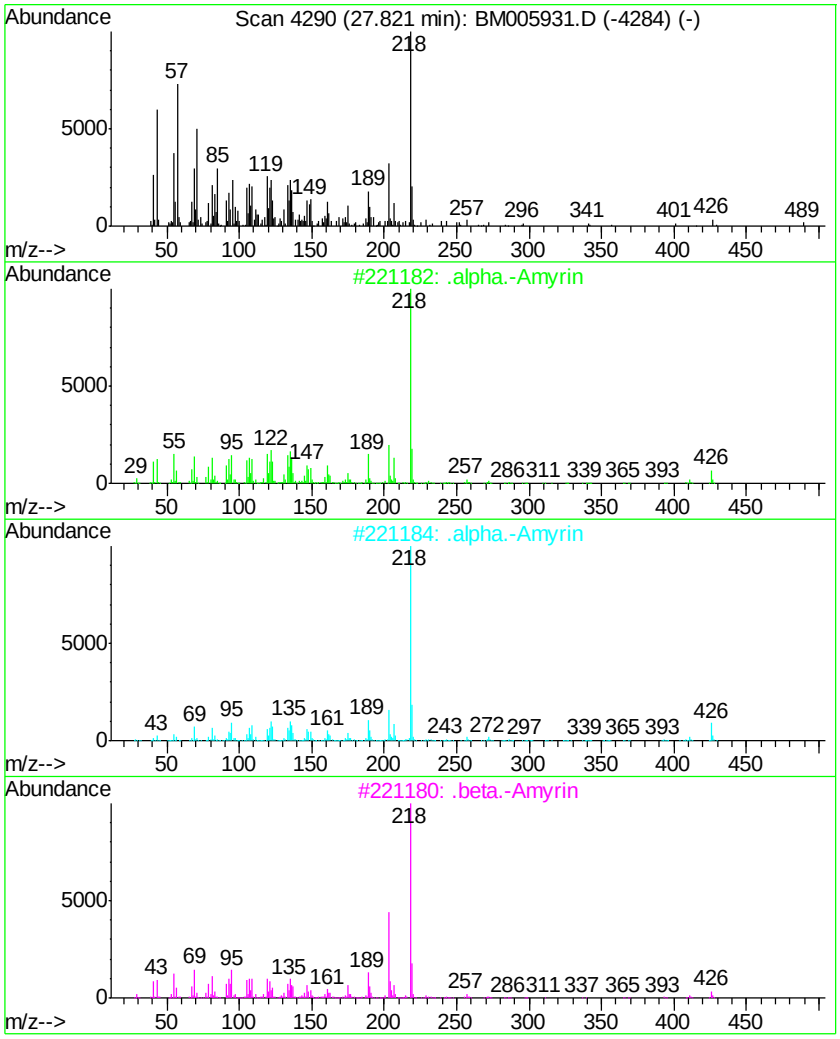
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

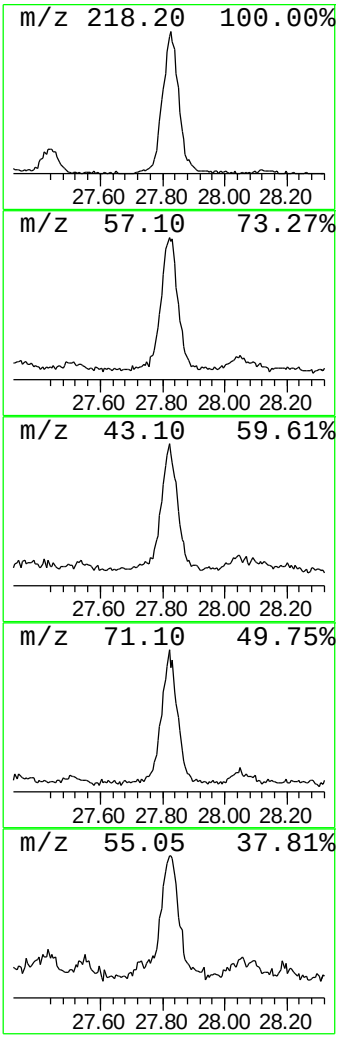
****

Peak Number 6 .alpha.-Amyrin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.82	2.85 ng/ul	1311900	Perylene-d12	23.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrin	426	C30H50O	000638-95-9	99
2	.alpha.-Amyrin	426	C30H50O	000638-95-9	92
3	.beta.-Amyrin	426	C30H50O	000559-70-6	86
4	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	70
5	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062216\
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Quant Title : SVOA 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
Trifluoroacetoxy ...	20.97	3.1	ng/ul	1444570	5	21.25	9278900	20.0
(DEL) Alkane: Str...	22.82	3.6	ng/ul	1643110	6	23.47	9212520	20.0
(DEL) Alkane: Str...	24.02	2.2	ng/ul	1017250	6	23.47	9212520	20.0
1H-Cycloprop[e]az...	27.04	6.4	ng/ul	2930260	6	23.47	9212520	20.0
.beta.-Amyrin	27.23	2.9	ng/ul	1333190	6	23.47	9212520	20.0
.alpha.-Amyrin	27.82	2.9	ng/ul	1311900	6	23.47	9212520	20.0