LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.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	6.322	562	567	572	rVB3	98065	159627	0.91%	0.141%
2	6.798	642	648	661	rVB2	881924	1591934	9.10%	1.411%
3	6.957	666	675	688	rVB2	663884	1309300	7.49%	1.160%
4	7.151	702	708	717	rBV	891602	1420844	8.12%	1.259%
5	7.616	781	787	797	rVB	1560801	2433538	13.91%	2.157%
6	7.757	809	811	817	rVB5	17550	25898	0.15%	0.023%
7	7.845	824	826	831	rVB5	19190	22970	0.13%	0.020%
8	8.328	901	908	921	rVB	886331	1427761	8.16%	1.265%
9	8.504	935	938	943	rVB5	15722	20855	0.12%	0.018%
10	8.763	975	982	995	rBV	821028	1389033	7.94%	1.231%
11	9.110	1035	1041	1049	rVB	569847	877387	5.02%	0.778%
12	9.234	1057	1062	1066	rBV3	20988	33541	0.19%	0.030%
13	9.281	1066	1070	1079	rVB	88893	144239	0.82%	0.128%
14	9.481	1095	1104	1112	rBV	637123	1088712	6.22%	0.965%
15	10.022	1188	1196	1214	rBV	1064107	1782782	10.19%	1.580%
16	10.392	1252	1259	1269	rBV	2075192	3499024	20.01%	3.101%
17	10.534	1275	1283	1292	rBV	793510	1416111	8.10%	1.255%
18	10.598	1292	1294	1306	rVB5	45107	73473	0.42%	0.065%
19	10.916	1344	1348	1354	rVB7	9527	18426	0.11%	0.016%
20	11.298	1406	1413	1417	rBV7	12930	22551	0.13%	0.020%
21	11.992	1525	1531	1539	rVB6	18864	36887	0.21%	0.033%
22	13.180	1726	1733	1742	rVB2	71118	129275	0.74%	0.115%
23	13.680	1812	1818	1822	rBV	1969002	2744852	15.69%	2.432%
24	13.727	1822	1826	1833	rVB	1139550	1547637	8.85%	1.371%
25	13.951	1856	1864	1872	rBV	2188390	3295737	18.84%	2.921%
26	14.263	1910	1917	1926	rBV	3029402	4579784	26.18%	4.058%
27	14.480	1947	1954	1971	rBV	493138	1002638	5.73%	0.889%
28	14.598	1971	1974	1976	rVV3	20447	28885	0.17%	0.026%
29	14.627	1976	1979	1986	rVV6	27521	51825	0.30%	0.046%
30	14.698	1986	1991	1998	rVB4	70225	115563	0.66%	0.102%
31	14.910	2021	2027	2031	rVB8	11490	19930	0.11%	0.018%
32	15.092	2055	2058	2063	rBV5	13551	17593	0.10%	0.016%
33	15.263	2080	2087	2096	rBV	2832869	4112875	23.51%	3.645%
34	15.386	2102	2108	2118	rBV	573575	828575	4.74%	0.734%

LSC Area Percent Report

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Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Title : SVOA CALIBRATION

35	15.504	2123	2128	2133	rVV	35155	54839	0.31%	0.049%
36	15.968	2202	2207	2211	rBV7	9887	19674	0.11%	0.017%
37	16.045	2217	2220	2224	rVB6	13576	19067	0.11%	0.017%
38	16.533	2298	2303	2306	rVV2	43617	59116	0.34%	0.052%
39	16.563	2306	2308	2314	rVB2	24112	34806	0.20%	0.031%
40	16.804	2345	2349	2354	rBV7	13838	23470	0.13%	0.021%
41	17.010	2378	2384	2395	rBV2	3683121	5269572	30.13%	4.670%
42	17.110	2395	2401	2411	rVV	3219136	4419035	25.27%	3.916%
43	17.263	2425	2427	2433	rVB7	22303	34120	0.20%	0.030%
44	17.427	2452	2455	2462	rVB8	20787	30210	0.17%	0.027%
45	17.868	2525	2530	2535	rBV	172191	225304	1.29%	0.200%
46	17.927	2536	2540	2548	rBV3	101196	160878	0.92%	0.143%
47	18.227	2586	2591	2597	rBV4	160258	235370	1.35%	0.209%
48	18.321	2603	2607	2611	rVB6	32489	44039	0.25%	0.039%
49	18.798	2686	2688	2693	rBV6	22171	30297	0.17%	0.027%
50	18.880	2698	2702	2707	rVV5	50355	98921	0.57%	0.088%
51	19.045	2727	2730	2736	rBV3	32672	50854	0.29%	0.045%
52	19.139	2742	2746	2750	rVB7	89665	121784	0.70%	0.108%
53	19.221	2757	2760	2764	rBV4	26415	32383	0.19%	0.029%
54	19.280	2767	2770	2771	rBV2	38355	41681	0.24%	0.037%
55	19.339	2777	2780	2785	rBV5	32987	53829	0.31%	0.048%
56	19.409	2786	2792	2798	rVV2	3916257	5399956	30.87%	4.785%
57	19.456	2798	2800	2804	rVB3	53077	58911	0.34%	0.052%
58	19.868	2866	2870	2874	rBV	291410	343868	1.97%	0.305%
59	19.992	2888	2891	2899	rVB	112455	145691	0.83%	0.129%
60	20.133	2911	2915	2924	rVB	356786	591780	3.38%	0.524%
61	20.309	2942	2945	2948	rBV4	86783	118567	0.68%	0.105%
62	20.368	2953	2955	2958	rVV4	63865	68357	0.39%	0.061%
63	20.451	2964	2969	2973	rBV	824835	1016545	5.81%	0.901%
64	20.827	3029	3033	3036	rBV	365845	466041	2.66%	0.413%
65	20.868	3036	3040	3047	rVB	448402	643630	3.68%	0.570%
66	20.951	3050	3054	3059	rBV	1018176	1323948	7.57%	1.173%
67	21.209	3091	3098	3107	rBV	4739850	6390770	36.54%	5.663%
68	21.392	3126	3129	3132	rBV	259624	268151	1.53%	0.238%
69	21.821	3198	3202	3210	rBV	2026991	2605753	14.90%	2.309%
70	22.274	3276	3279	3283	rBV	426208	543959	3.11%	0.482%
71	22.315	3284	3286	3291	rVB2	347144	428919	2.45%	0.380%

LSC Area Percent Report

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Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Title : SVOA CALIBRATION

72	22.497	3314	3317	3322	rVB	377529	476957	2.73%	0.423%
73	22.774	3360	3364	3368	rBV	1039171	1413319	8.08%	1.252%
74	23.262	3441	3447	3454	rBV	3200106	5748578	32.87%	5.094%
75	23.333	3456	3459	3463	rVV	499167	712775	4.08%	0.632%
76	23.397	3464	3470	3483	rVB2	3851146	7302272	41.75%	6.471%
77	23.633	3507	3510	3517	rVB2	529485	833371	4.76%	0.739%
78	26.780	4036	4045	4054	rBV3	3321805	10124001	57.88%	8.972%
79	27.285	4122	4131	4151	rVB3	4899314	17490473	100.00%	15.499%

Sum of corrected areas: 112845903

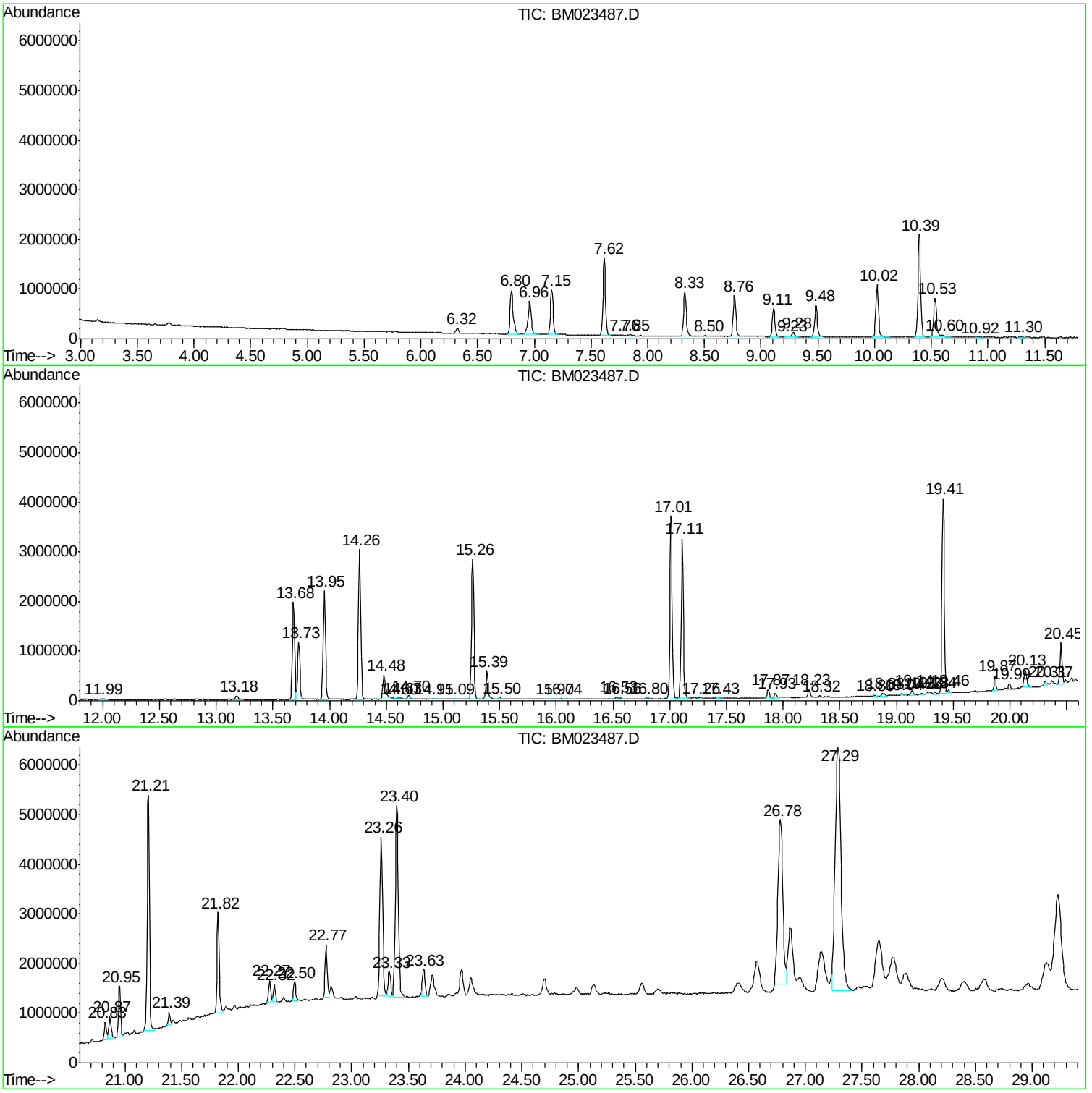
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

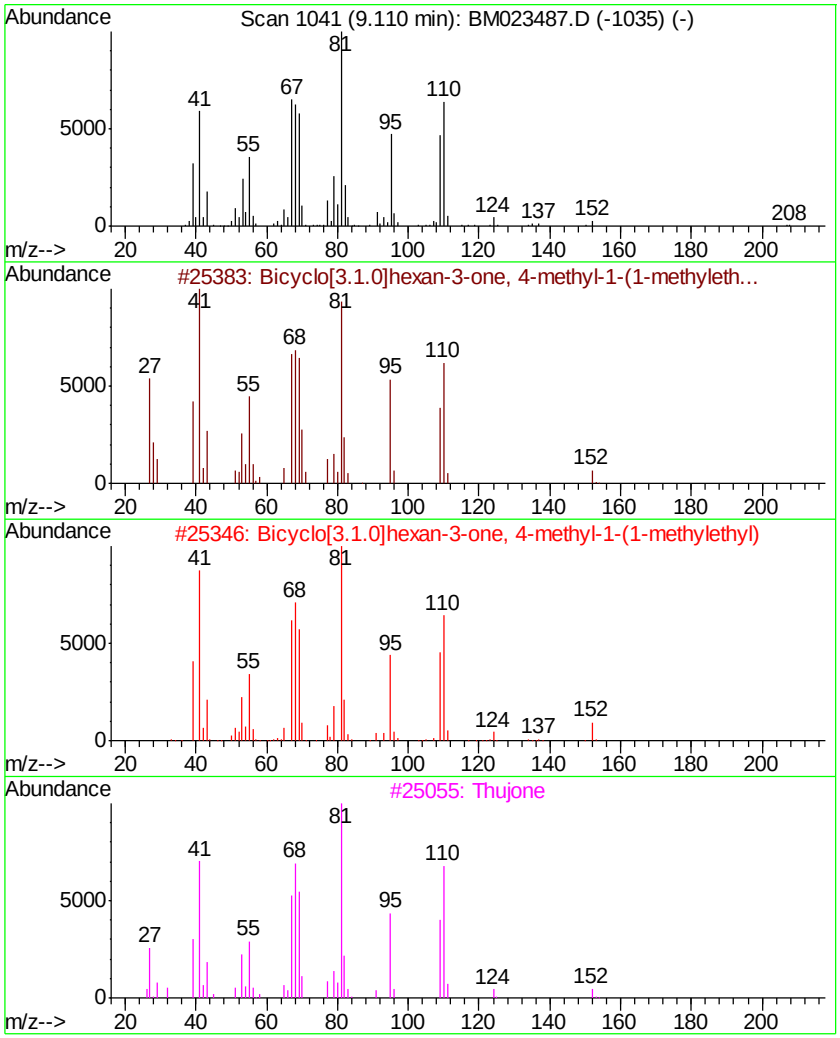
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

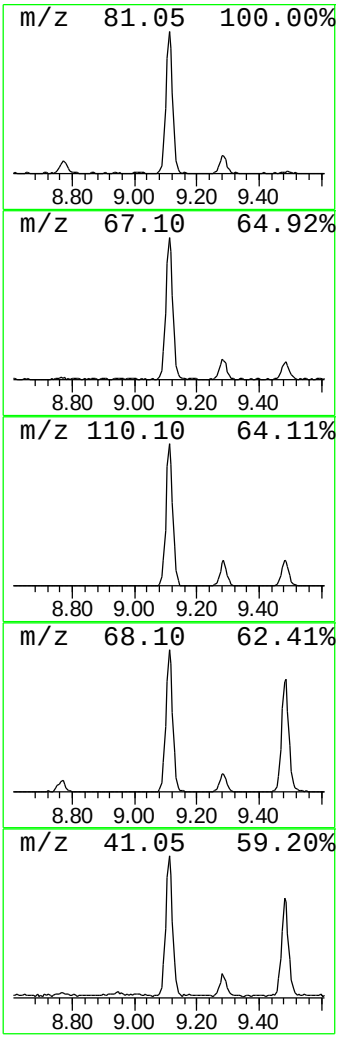
****

Peak Number 1 Bicyclo[3.1.0]hexan-3-one, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.11	5.02 ng/ul	877387	Naphthalene-d8	10.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	000471-15-8	93
2	Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	91
3	Thujone	152	C10H16O	000546-80-5	90
4	Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	80
5	3,5-Octadiene, (Z,Z)-	110	C8H14	007348-80-3	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

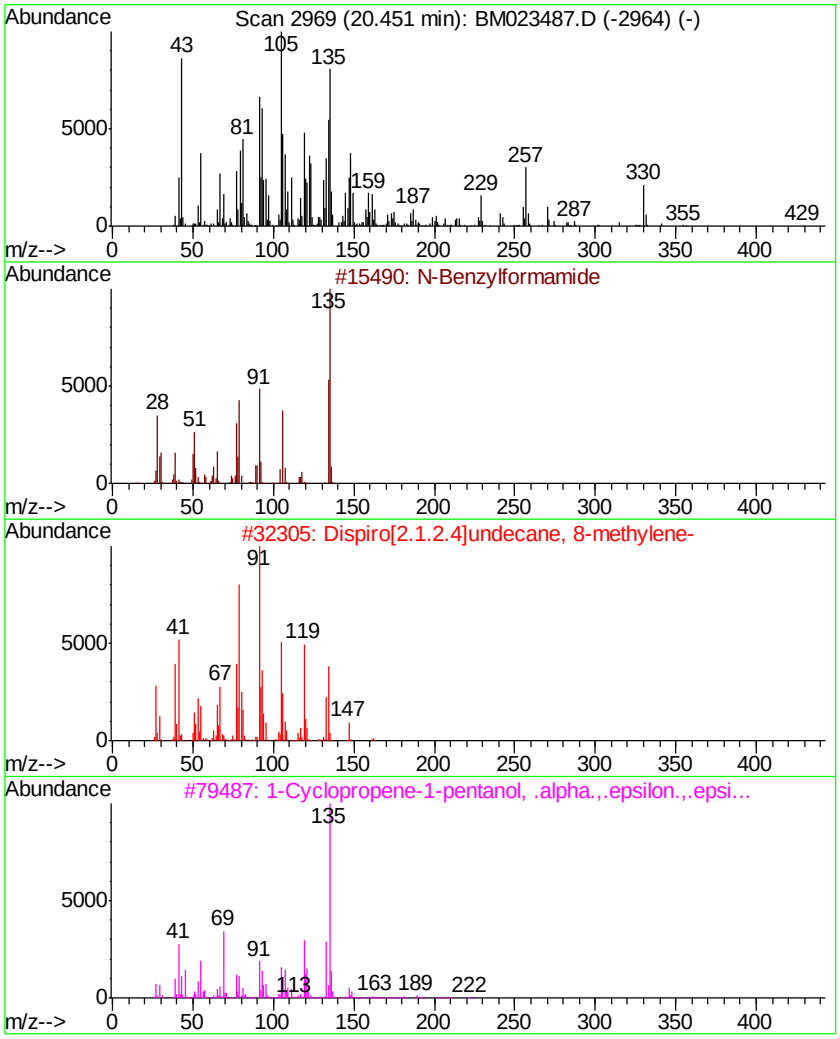
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

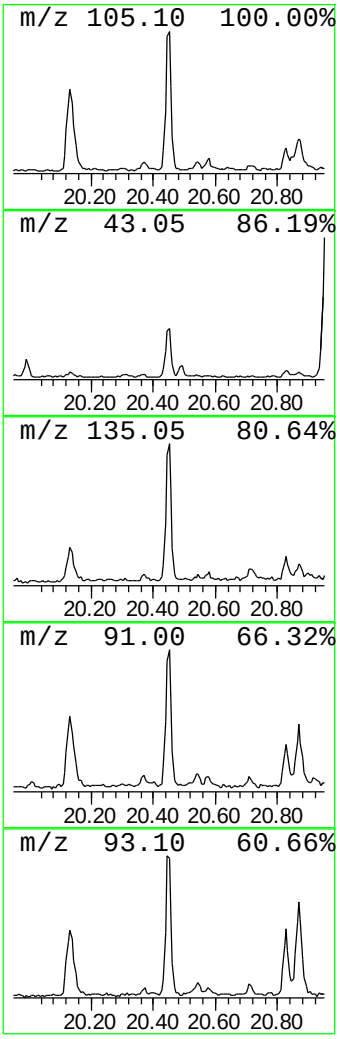
****

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	3.18 ng/ul	1016550	Chrysene-d12	21.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Benzylformamide	135	C8H9NO	006343-54-0	43
2	Dispiro[2.1.2.4]undecane, 8-meth...	162	C12H18	051567-08-9	38
3	1-Cyclopropene-1-pentanol, .alph...	222	C15H26O	090165-06-3	38
4	Bicyclo[3.2.1]oct-2-ene, 3-methy...	134	C10H14	049826-53-1	30
5	N-Benzylformamide	135	C8H9NO	006343-54-0	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

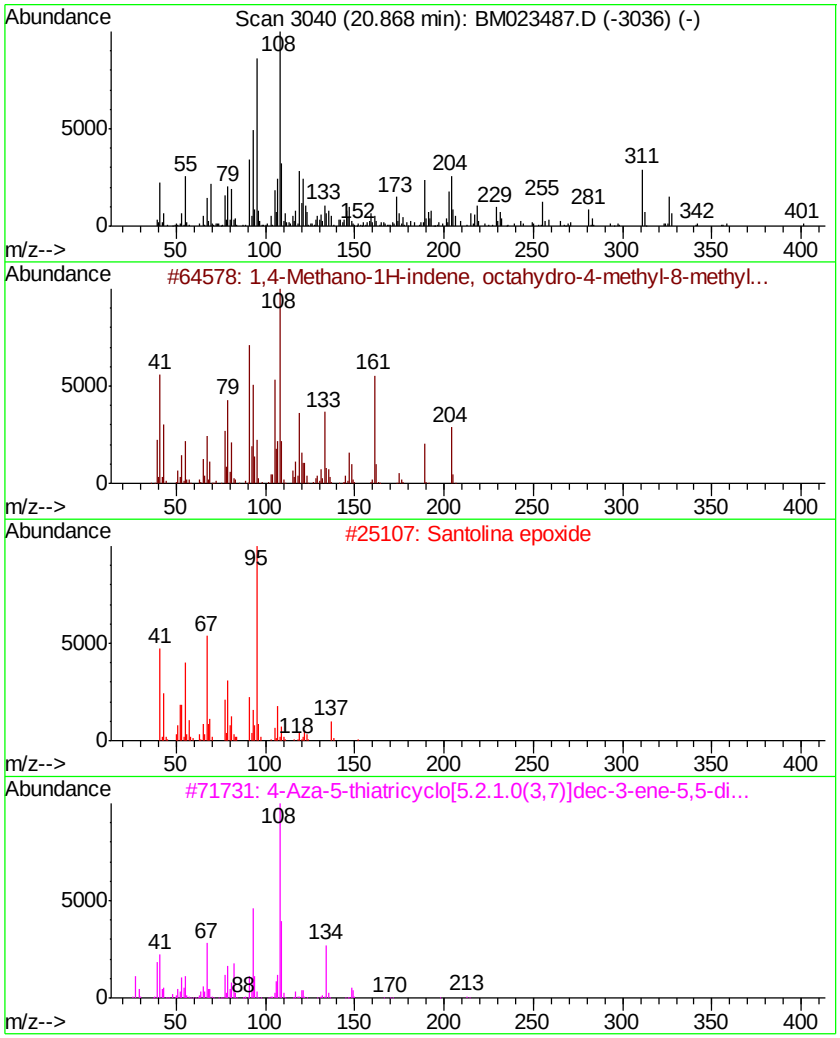
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

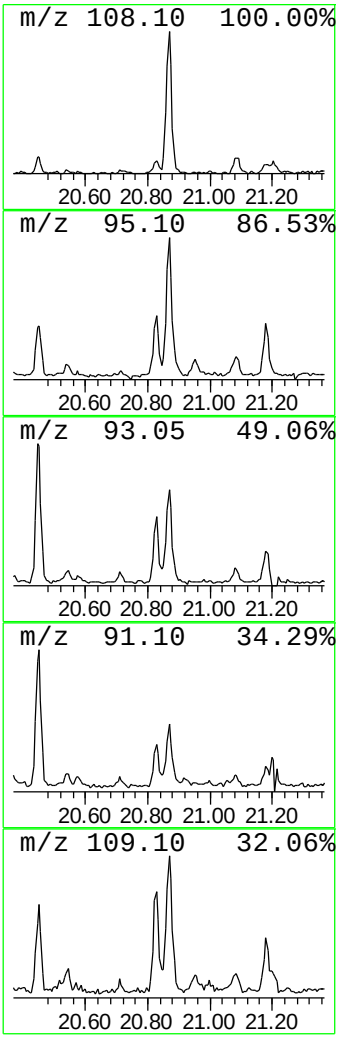
****

Peak Number 3 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	2.01 ng/ul	643630	Chrysene-d12	21.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Methano-1H-indene, octahydro...	204	C15H24	003650-28-0	49
2	Santolina epoxide	152	C10H16O	060485-45-2	30
3	4-Aza-5-thiatricyclo[5.2.1.0(3,7...	213	C10H15NO2S	104319-35-9	27
4	Fumaric acid, decyl 2-methylcycl...	364	C22H36O4	1000345-16-1	27
5	1-Cyclopenta-2,4-dienylundec-10-...	232	C16H24O	1000190-22-6	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

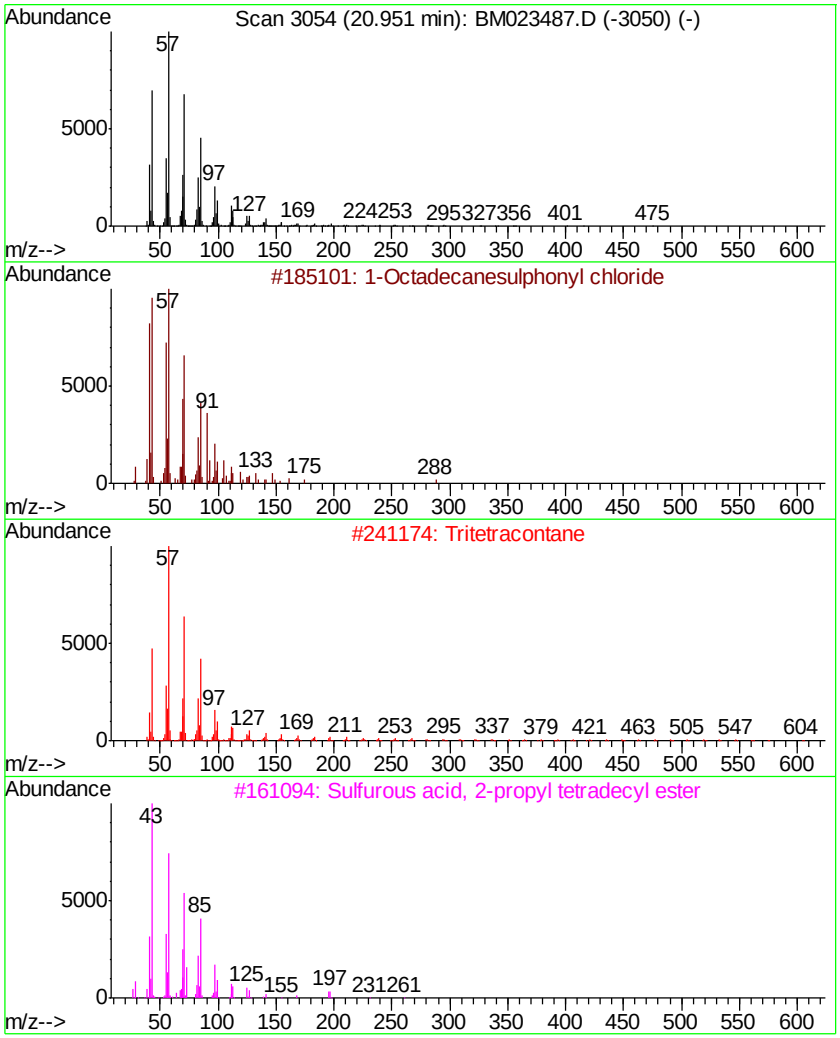
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

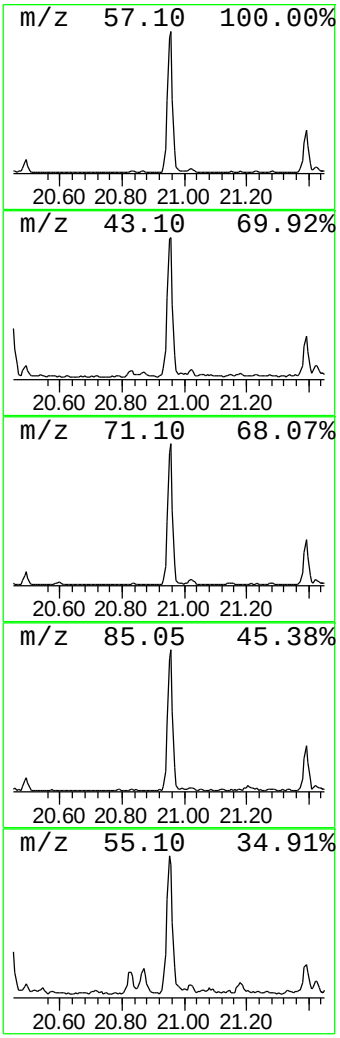
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Octadecanesulphonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	4.14 ng/ul	1323950	Chrysene-d12	21.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2	Tritetracontane	605	C43H88	007098-21-7	91
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	91
5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

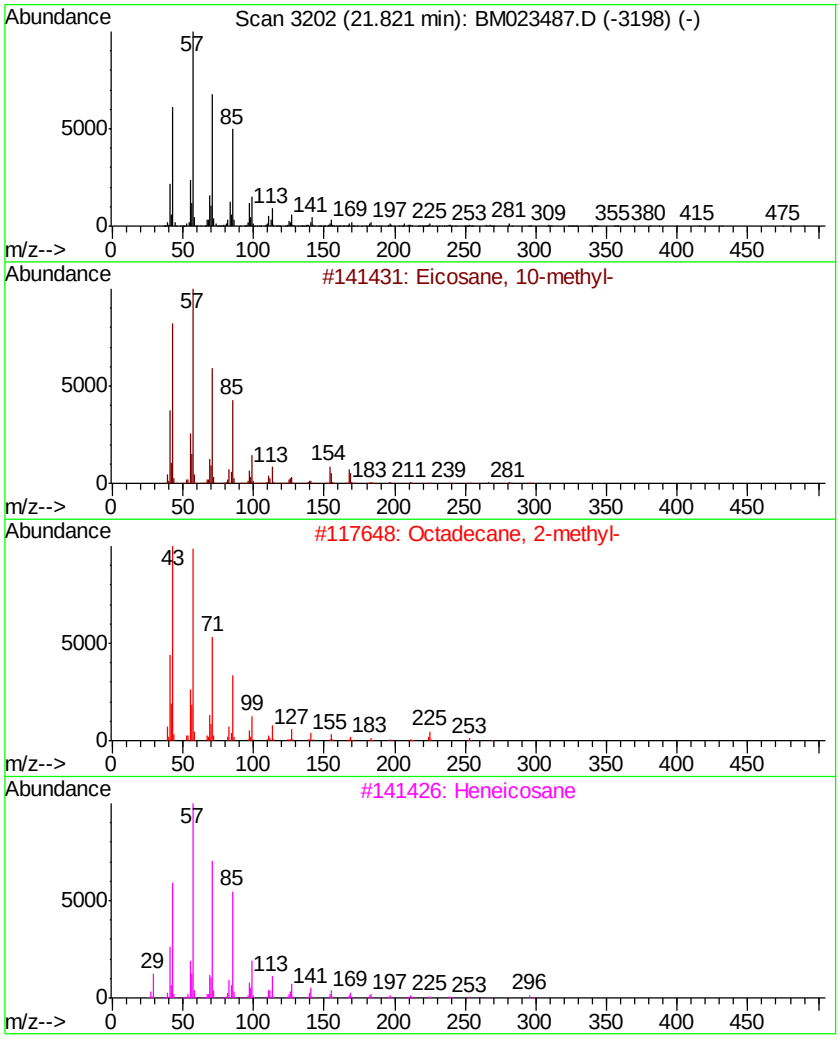
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

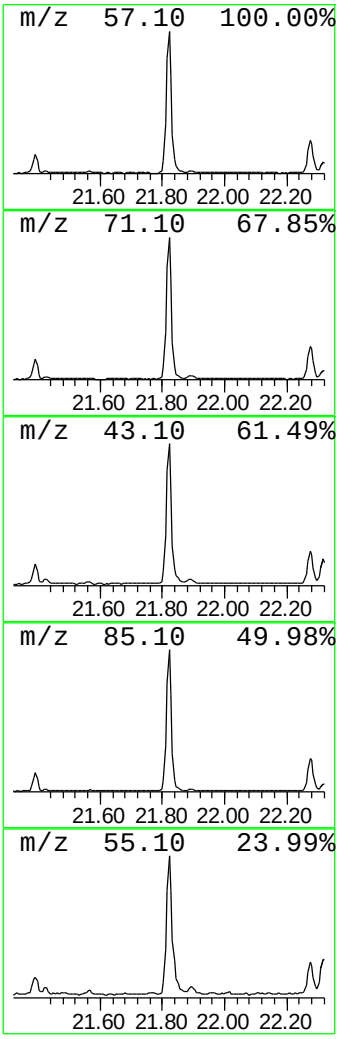
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.82	8.15 ng/ul	2605750	Chrysene-d12	21.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

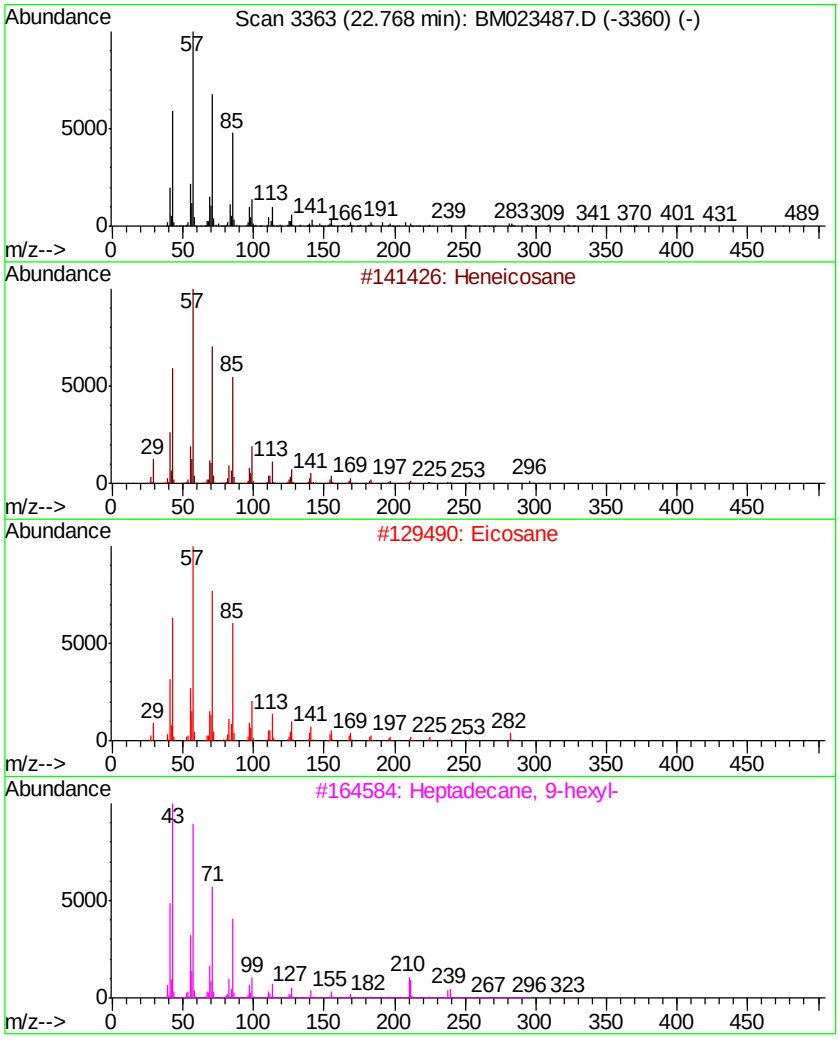
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

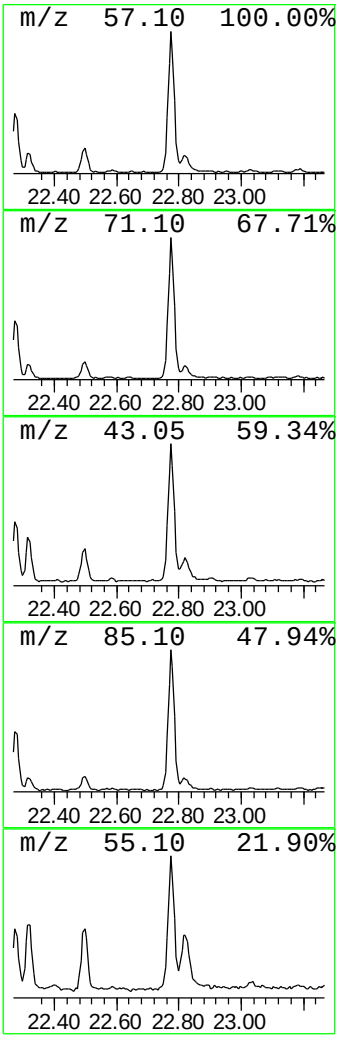
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	3.87 ng/ul	1413320	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane	282	C20H42	000112-95-8	97
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
4	Tricosane	324	C23H48	000638-67-5	93
5	Eicosane	282	C20H42	000112-95-8	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

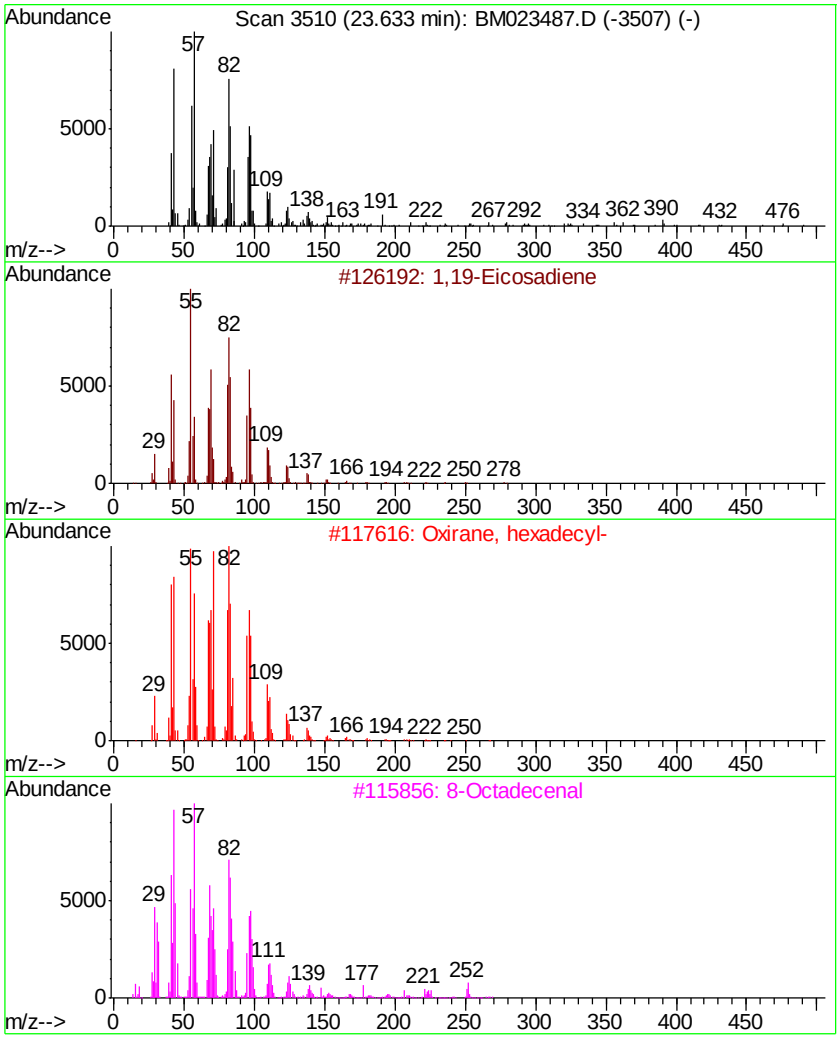
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

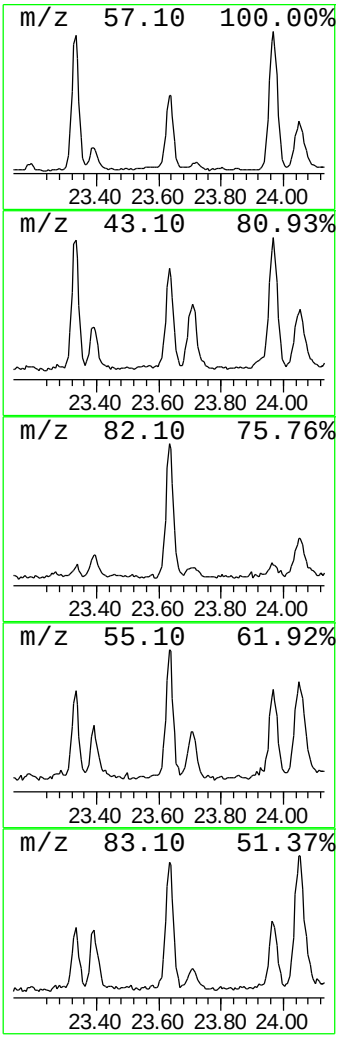
****

Peak Number 7 1,19-Eicosadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.63	2.28 ng/ul	833371	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	8-Octadecenal	266	C18H34O	056554-94-0	90
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
Quant Title : SVOA CALIBRATION

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

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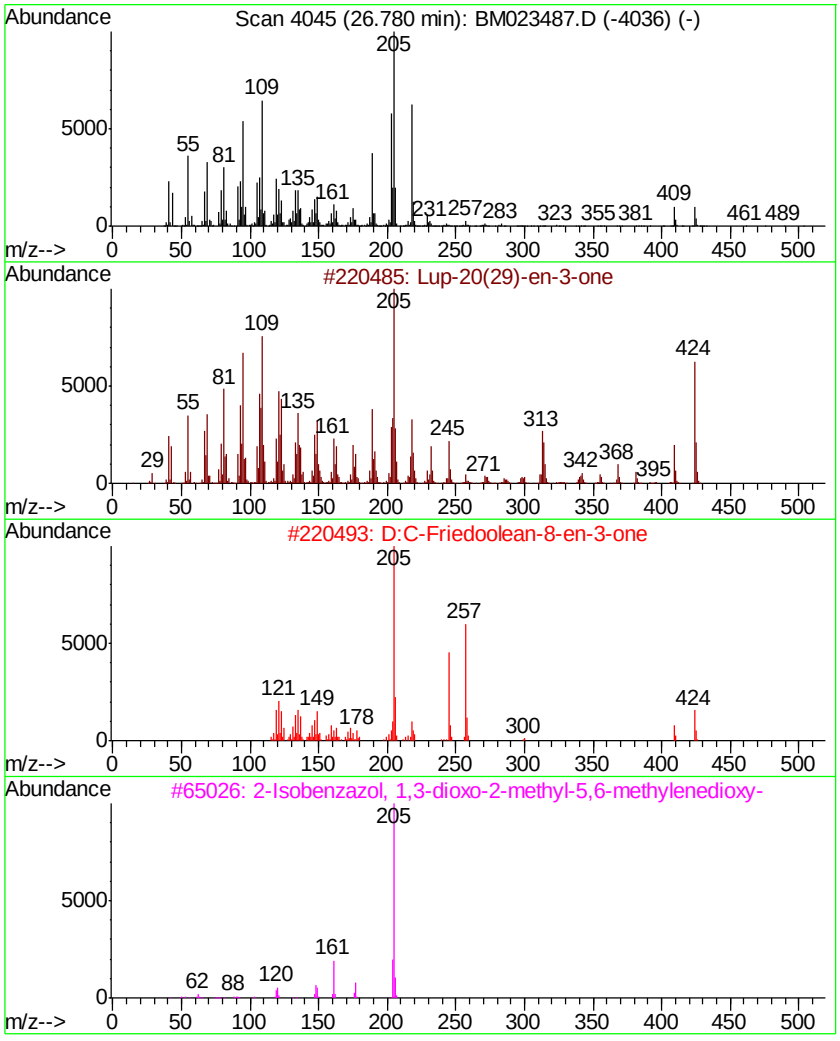
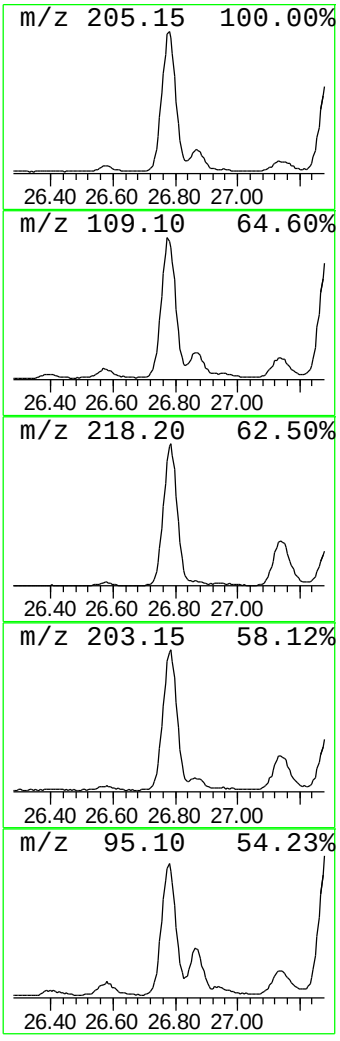
Peak Number 8 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.78	27.73 ng/ul	10124000	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	62
2	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	46
3	2-Isobenzazol, 1,3-dioxo-2-methy...	205	C10H7NO4	114252-71-0	25
4	6-Phenylisoquinoline	205	C15H11N	070125-61-0	22
5	5-(1H-Pyrrol-3-ylmethylene)-pyri...	205	C9H7N3O3	1000318-16-3	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102919\
Data File : BM023487.D
Acq On : 30 Oct 2019 18:15
Operator : JU
Sample : K5434-14
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNH5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102319MA.M
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
Bicyclo[3.1.0]hex...	9.11	5.0	ng/ul	877387	2	10.39	3499020	20.0
unknown-01	20.45	3.2	ng/ul	1016550	5	21.21	6390770	20.0
unknown-02	20.87	2.0	ng/ul	643630	5	21.21	6390770	20.0
1-Octadecanesulph...	20.95	4.1	ng/ul	1323950	5	21.21	6390770	20.0
(DEL) Alkane: Str...	21.82	8.2	ng/ul	2605750	5	21.21	6390770	20.0
(DEL) Alkane: Str...	22.77	3.9	ng/ul	1413320	6	23.40	7302270	20.0
1,19-Eicosadiene	23.63	2.3	ng/ul	833371	6	23.40	7302270	20.0
Lup-20(29)-en-3-one	26.78	27.7	ng/ul	10124000	6	23.40	7302270	20.0