LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

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-BM121719MA.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	2.993	16	18	29	rVB	71743	109379	1.74%	0.165%
2	6.593	626	630	633	rBV3	11101	16928	0.27%	0.026%
3	6.634	633	637	654	rVB	176404	354169	5.64%	0.535%
4	6.787	658	663	678	rBV	782543	1298332	20.66%	1.959%
5	6.975	688	695	712	rVB	809193	1360550	21.66%	2.053%
6	7.434	765	773	787	rBV	897409	1467865	23.36%	2.215%
7	8.157	890	896	910	rBV	570331	1022423	16.27%	1.543%
8	8.587	962	969	990	rBV	926102	1639846	26.10%	2.475%
9	9.022	1038	1043	1048	rVB	24120	34237	0.54%	0.052%
10	9.304	1084	1091	1108	rBV	750207	1310424	20.86%	1.978%
11	9.839	1176	1182	1201	rBV	918472	1914844	30.48%	2.890%
12	10.198	1237	1243	1254	rBV	1302743	2186528	34.80%	3.300%
13	10.386	1269	1275	1287	rBV3	22929	68900	1.10%	0.104%
14	11.510	1462	1466	1473	rVB3	11508	15888	0.25%	0.024%
15	11.828	1515	1520	1528	rVB3	11180	23144	0.37%	0.035%
16	13.522	1802	1808	1814	rBV	2434973	3423817	54.49%	5.167%
17	13.569	1814	1816	1828	rVB	146313	212844	3.39%	0.321%
18	13.786	1846	1853	1872	rBV	2705729	3970100	63.19%	5.992%
19	14.098	1899	1906	1919	rBV	2082880	3026826	48.18%	4.568%
20	14.374	1947	1953	1968	rBV2	40768	138876	2.21%	0.210%
21	14.933	2041	2048	2050	rBV5	4526	6495	0.10%	0.010%
22	15.098	2070	2076	2092	rBV	3532063	5210870	82.94%	7.864%
23	15.251	2096	2102	2114	rBV	902686	1373692	21.86%	2.073%
24	15.345	2114	2118	2122	rVB	40273	62991	1.00%	0.095%
25	15.851	2200	2204	2206	rBV3	5030	6643	0.11%	0.010%
26	15.892	2206	2211	2214	rVB4	11332	17062	0.27%	0.026%
27	16.651	2337	2340	2344	rVB4	9502	10711	0.17%	0.016%
28	16.851	2368	2374	2385	rBV	2433769	3502538	55.75%	5.286%
29	16.951	2385	2391	2406	rVV2	3820826	5507142	87.65%	8.311%
30	17.780	2526	2532	2542	rBV	114753	202595	3.22%	0.306%
31	17.898	2550	2552	2557	rVB6	6594	8785	0.14%	0.013%
32	18.898	2719	2722	2727	rBV	38471	56514	0.90%	0.085%
33	19.080	2748	2753	2757	rBV5	42698	71187	1.13%	0.107%
34	19.151	2761	2765	2768	rVV2	34618	44371	0.71%	0.067%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

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-BM121719MA.M
Title : SVOA CALIBRATION

35	19.262	2778	2784	2796	rBV	4581012	6202203	98.72%	9.360%
36	20.762	3034	3039	3043	rBV	281128	426862	6.79%	0.644%
37	20.809	3043	3047	3052	rVV2	923227	1311487	20.87%	1.979%
38	20.862	3052	3056	3064	rVV	1468793	1769803	28.17%	2.671%
39	20.933	3066	3068	3072	rVB	73239	81410	1.30%	0.123%
40	21.068	3086	3091	3105	rBV	2956052	3807123	60.60%	5.746%
41	21.250	3119	3122	3127	rBV	158190	154338	2.46%	0.233%
42	21.668	3190	3193	3200	rBV	206793	294592	4.69%	0.445%
43	22.109	3265	3268	3274	rVB	324327	384006	6.11%	0.580%
44	22.586	3346	3349	3356	rVB	424903	540741	8.61%	0.816%
45	23.068	3424	3431	3436	rBV	3568203	6282838	100.00%	9.482%
46	23.115	3436	3439	3446	rVV	518812	777785	12.38%	1.174%
47	23.197	3447	3453	3465	rVB	2154049	3914466	62.30%	5.908%
48	23.715	3538	3541	3548	rVB	384282	634612	10.10%	0.958%

Sum of corrected areas: 66259782

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
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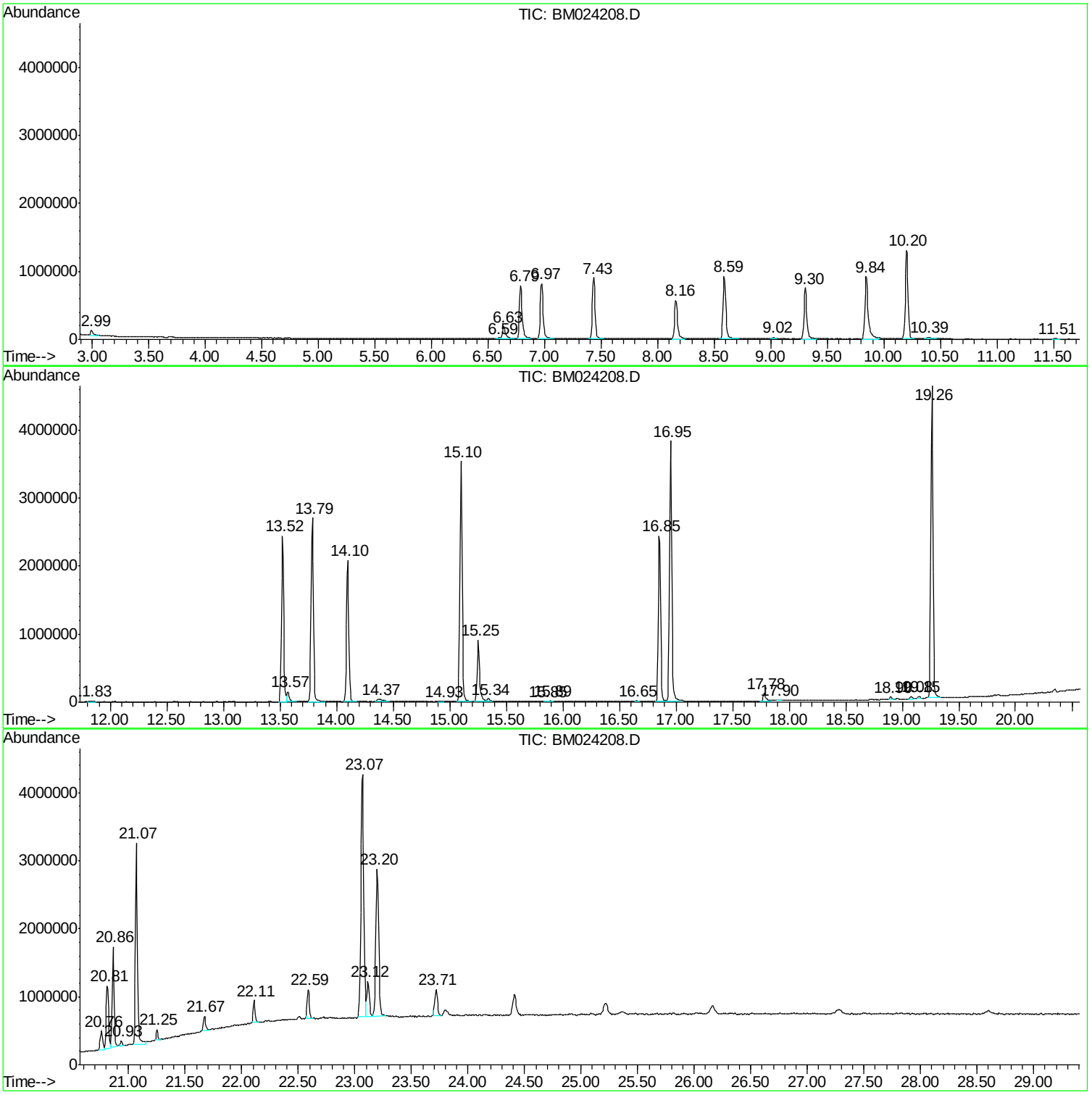
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

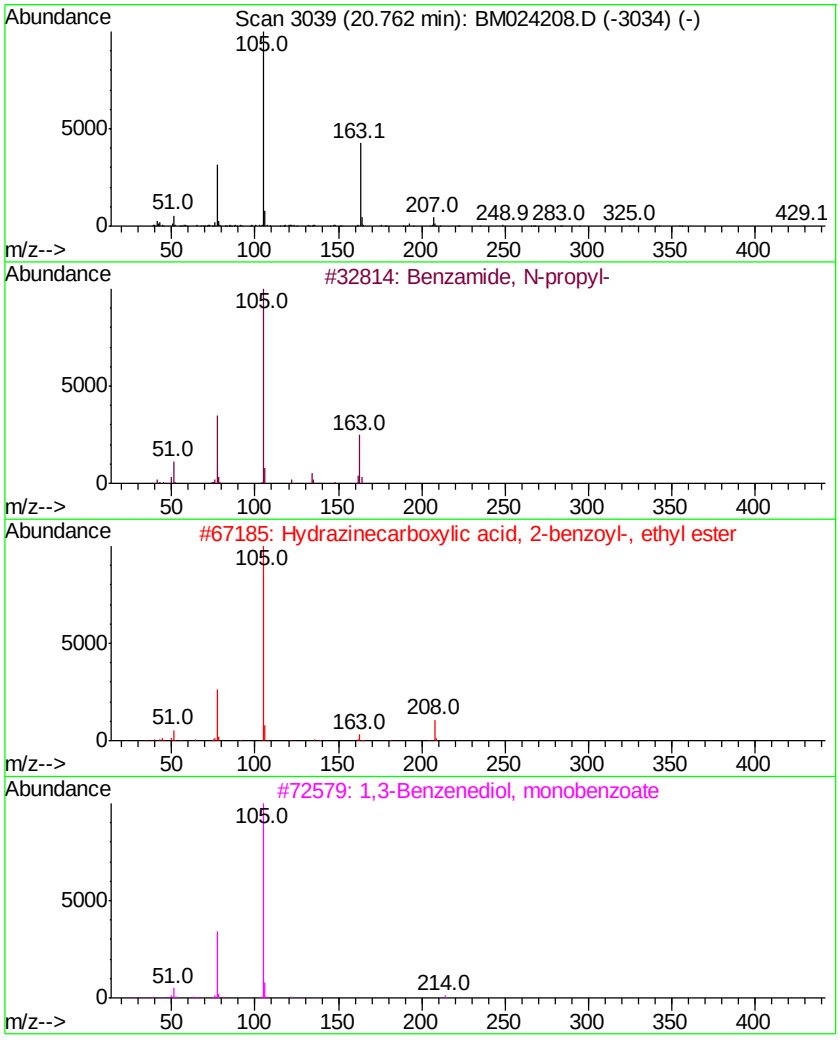
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

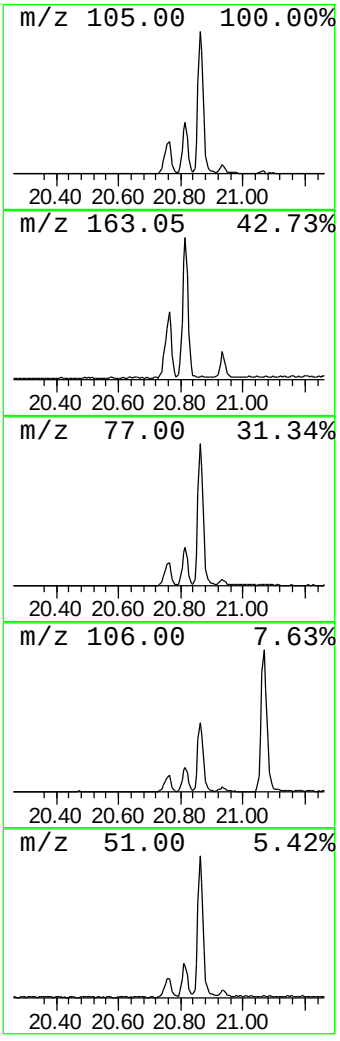
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzamide, N-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	2.24 ng/ul	426862	Chrysene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	50
2	Hydrazinecarboxylic acid, 2-benz...	208	C10H12N2O3	010465-97-1	35
3	1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	27
4	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	27
5	1,2-Dibenzoyl-1-methylhydrazine	254	C15H14N2O2	021150-15-2	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

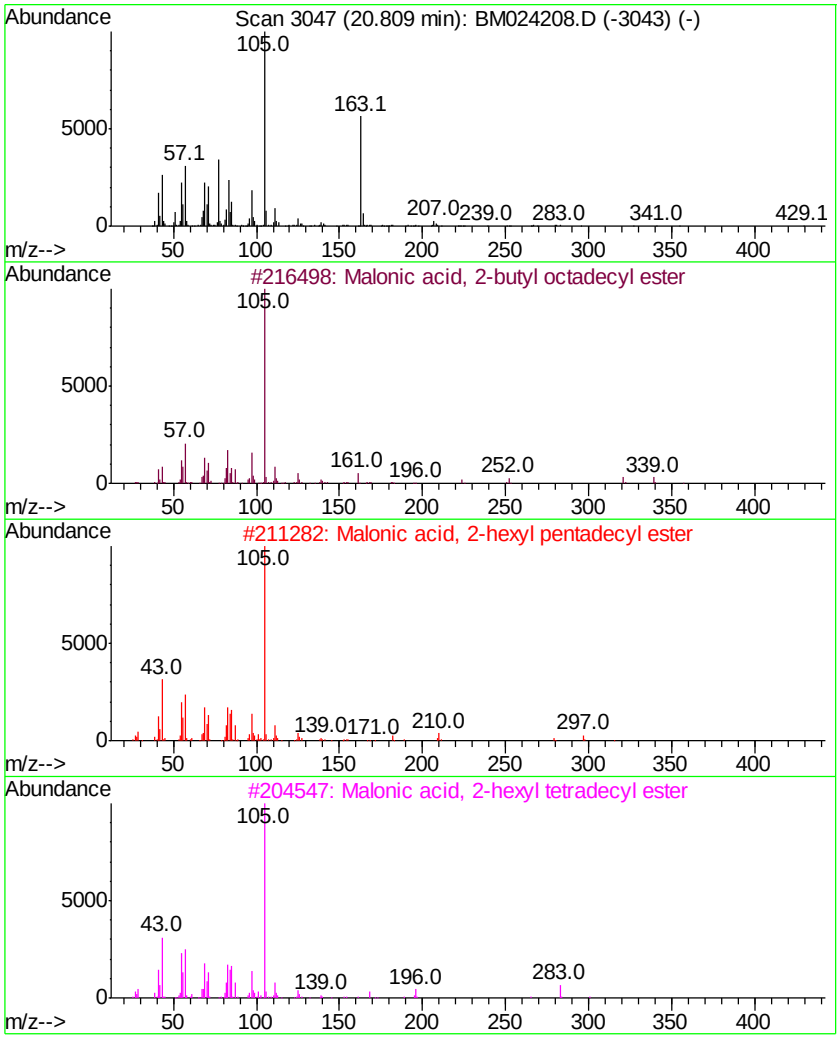
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

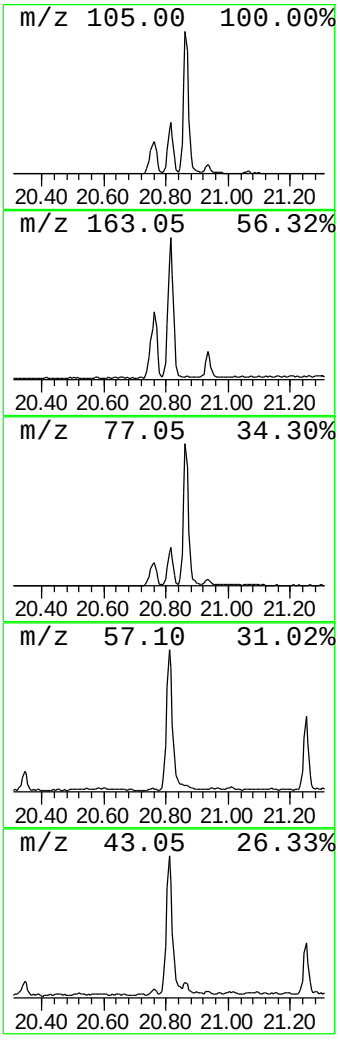
****

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	6.89 ng/ul	1311490	Chrysene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid, 2-butyl octadecyl ...	412	C25H48O4	1000349-08-4	43
2	Malonic acid, 2-hexyl pentadecyl...	398	C24H46O4	1000349-32-8	38
3	Malonic acid, 2-hexyl tetradecyl...	384	C23H44O4	1000349-32-7	35
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	35
5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

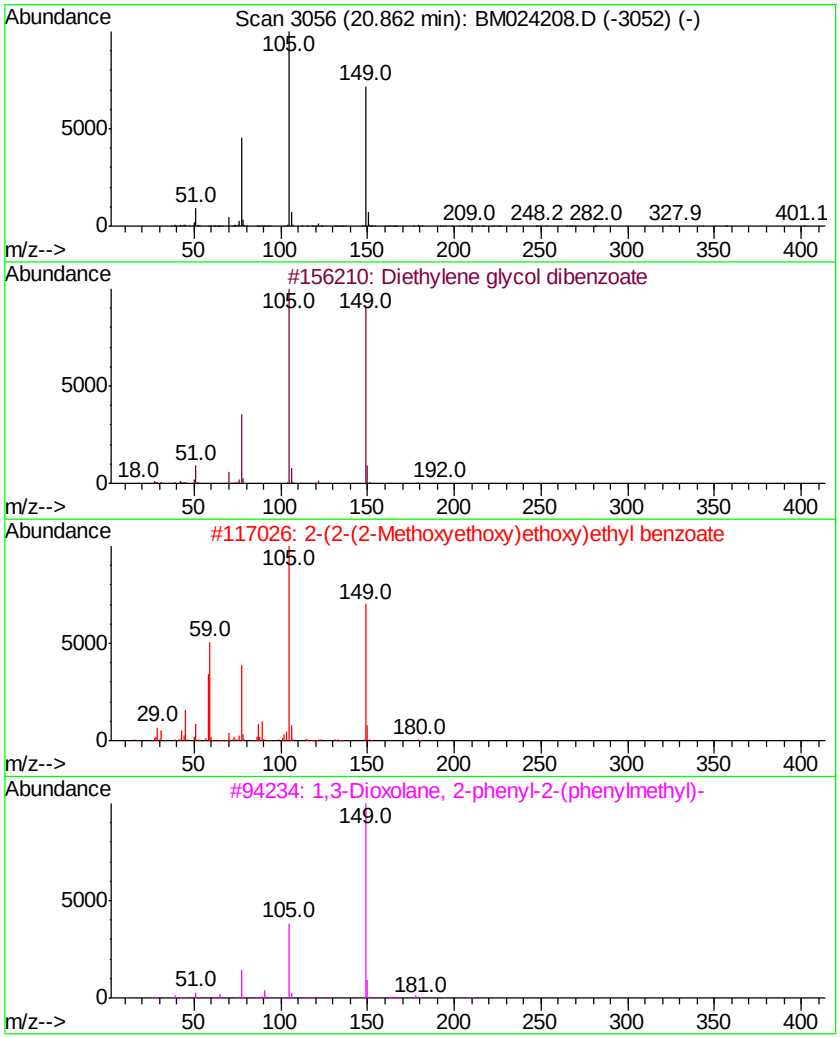
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

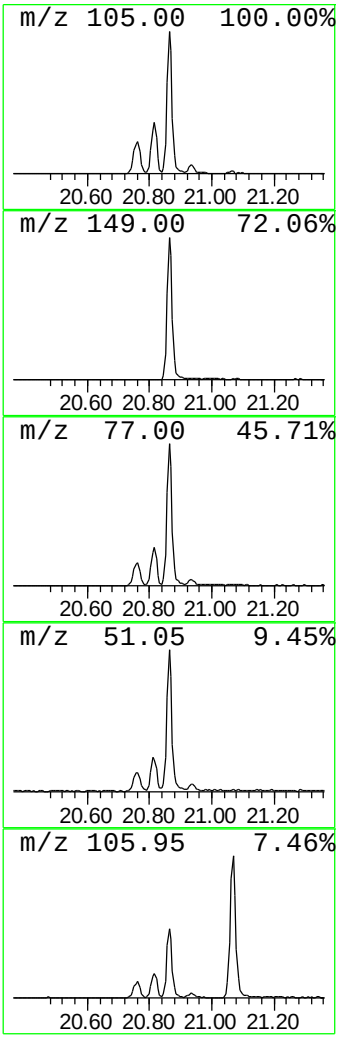
****

Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	9.30 ng/ul	1769800	Chrysene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
3	1,3-Dioxolane, 2-phenyl-2-(pheny...	240	C16H16O2	004362-19-0	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

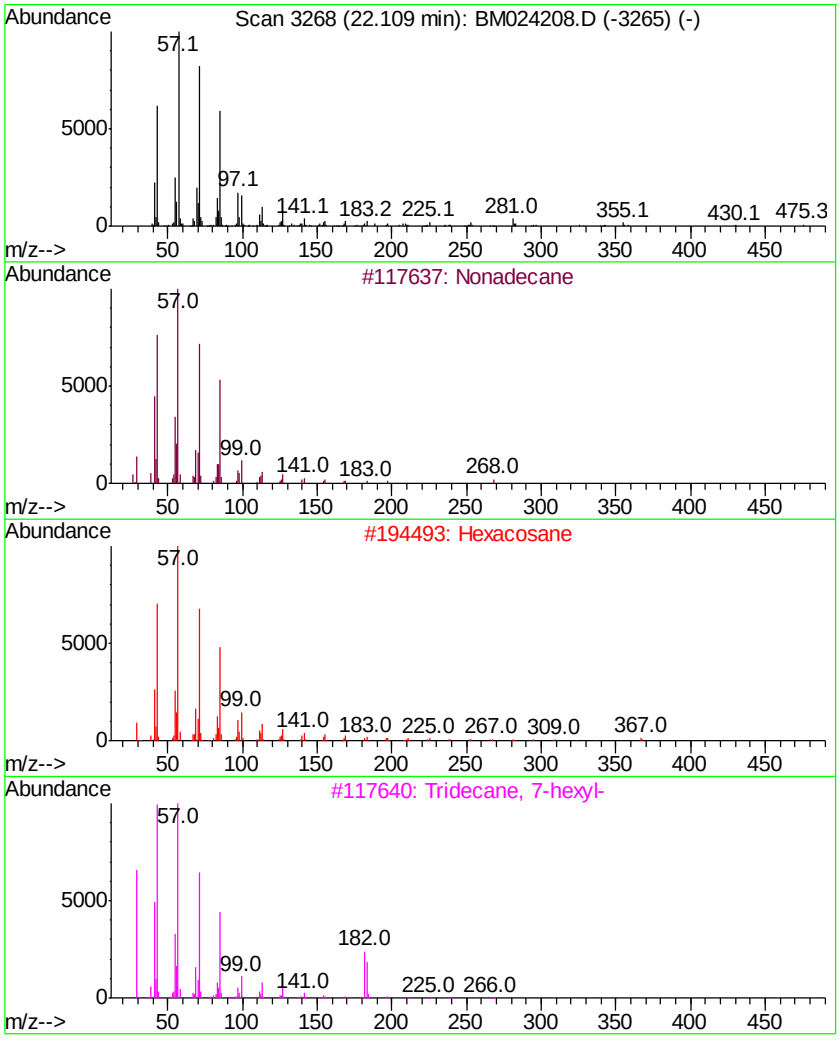
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

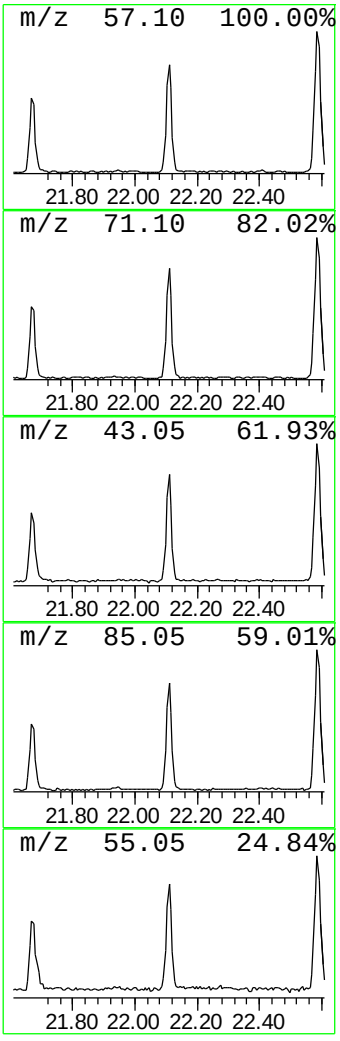
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	2.02 ng/ul	384006	Chrysene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

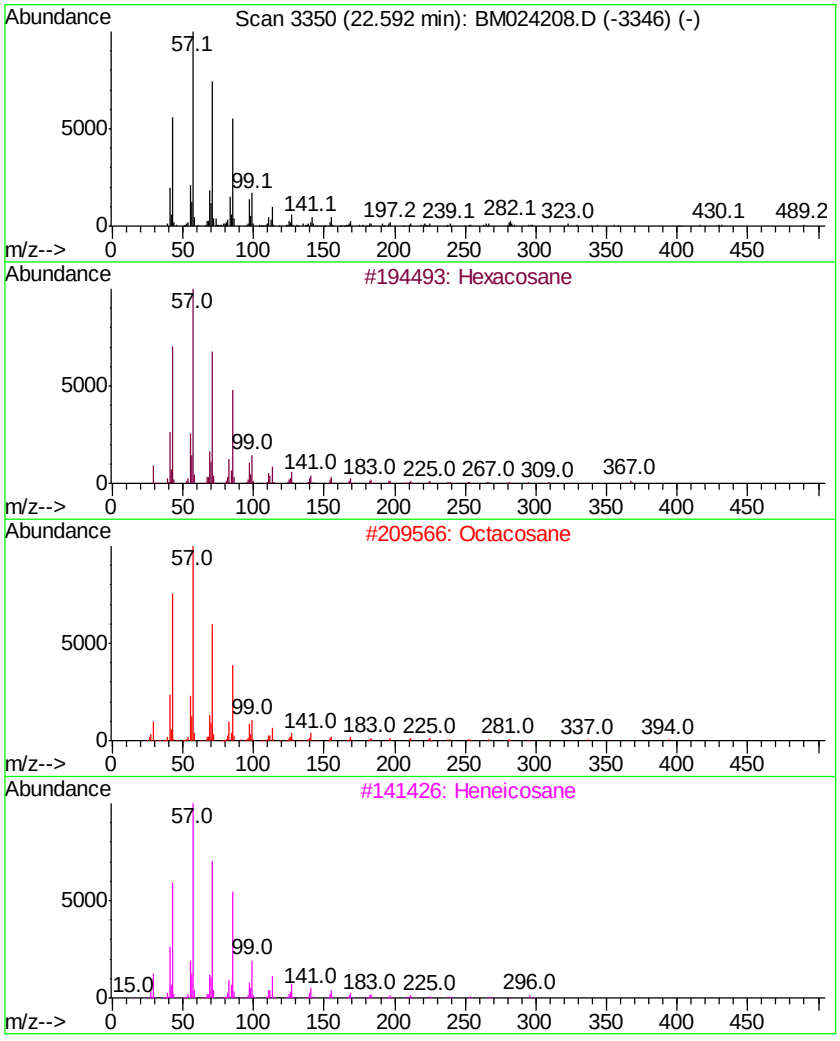
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

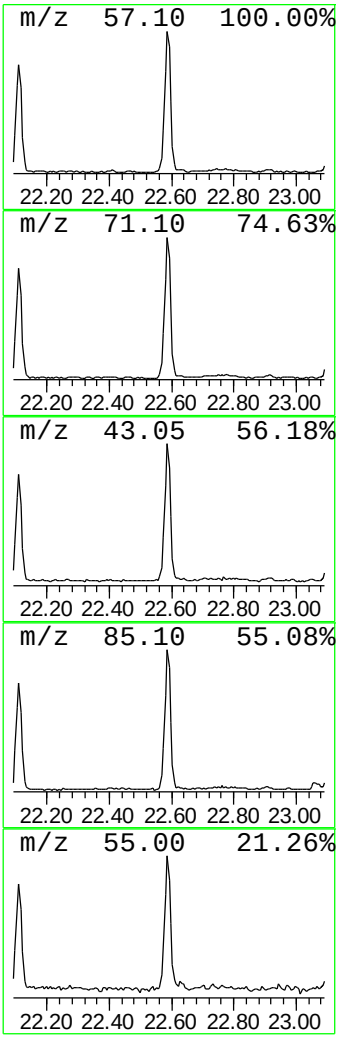
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.59	2.76 ng/ul	540741	Perylene-d12	23.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.M
Quant Title : SVOA CALIBRATION

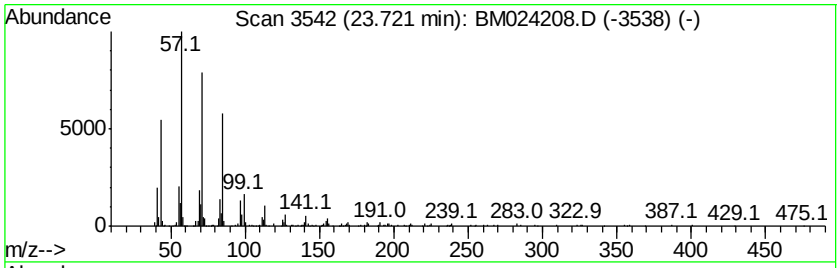
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

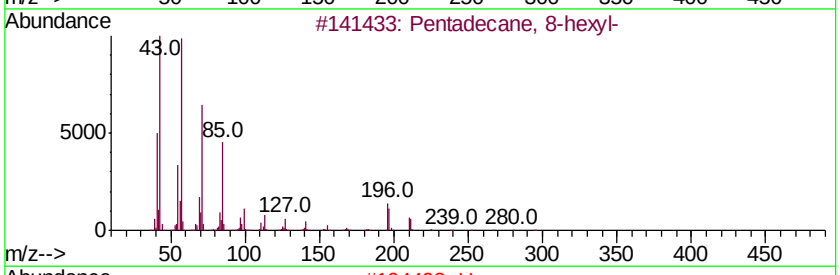
****

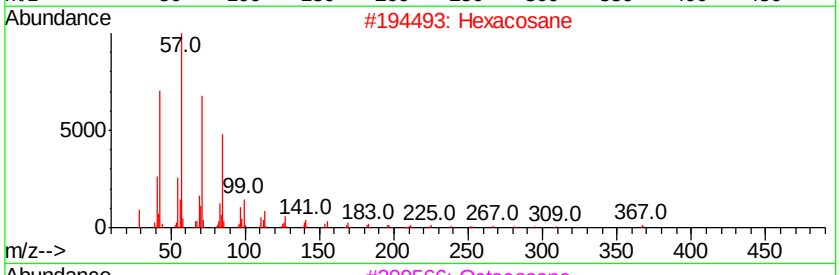
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

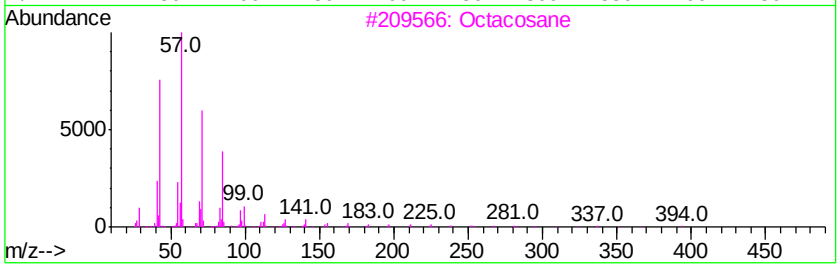
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.72	3.24 ng/ul	634612	Perylene-d12	23.20

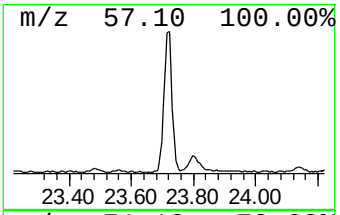
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Docosane, 5-butyl-	366	C26H54	055282-16-1	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86

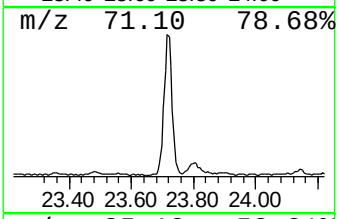


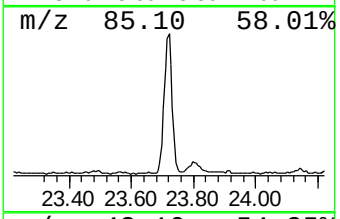


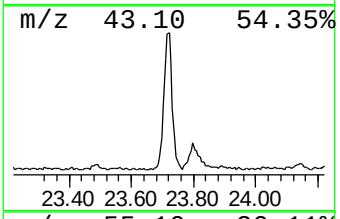


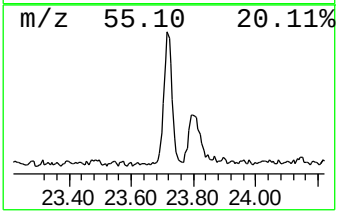












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121919\
Data File : BM024208.D
Acq On : 20 Dec 2019 17:51
Operator : JU
Sample : K6253-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0C24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM121719MA.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
Benzamide, N-propyl-	20.76	2.2	ng/ul	426862	5	21.07	3807120	20.0
unknown-01	20.81	6.9	ng/ul	1311490	5	21.07	3807120	20.0
Diethylene glycol...	20.86	9.3	ng/ul	1769800	5	21.07	3807120	20.0
(DEL) Alkane: Str...	22.11	2.0	ng/ul	384006	5	21.07	3807120	20.0
(DEL) Alkane: Str...	22.59	2.8	ng/ul	540741	6	23.20	3914470	20.0
(DEL) Alkane: Str...	23.72	3.2	ng/ul	634612	6	23.20	3914470	20.0