LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN032318\
Data File : BN000589.D
Acq On : 23 Mar 2018 21:42
Operator : JU/SJ
Sample : J1986-22
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : BEEL3

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:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.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	3.590	21	26	36	rVB2	48676	85976	1.88%	0.183%
2	4.302	143	147	152	rBV2	3067	5252	0.12%	0.011%
3	4.420	162	167	171	rVB3	4602	6850	0.15%	0.015%
4	4.767	222	226	230	rBV2	3337	5218	0.11%	0.011%
5	4.808	230	233	237	rVB2	3767	4786	0.10%	0.010%
6	5.408	329	335	344	rVB	93322	142218	3.12%	0.302%
7	6.178	459	466	470	rBV2	5184	8061	0.18%	0.017%
8	6.419	499	507	514	rBV	10784	19173	0.42%	0.041%
9	6.566	527	532	538	rVB2	4659	7590	0.17%	0.016%
10	7.549	693	699	711	rVB	250872	415667	9.10%	0.884%
11	7.713	720	727	737	rBV	776329	1252012	27.42%	2.663%
12	7.813	740	744	750	rVB2	4135	7411	0.16%	0.016%
13	7.931	757	764	772	rBV	781158	1296272	28.39%	2.757%
14	7.996	772	775	781	rVB3	3798	5198	0.11%	0.011%
15	8.408	839	845	851	rBV	657437	1087446	23.82%	2.313%
16	8.455	851	853	859	rVB2	17594	22709	0.50%	0.048%
17	8.943	932	936	944	rVB	14988	25319	0.55%	0.054%
18	9.119	959	966	976	rBV	693717	1139665	24.96%	2.424%
19	9.237	983	986	993	rVB3	4068	7380	0.16%	0.016%
20	9.513	1028	1033	1039	rBV	22027	34783	0.76%	0.074%
21	9.590	1039	1046	1056	rBV	868053	1454824	31.87%	3.094%
22	10.319	1162	1170	1182	rVB	719473	1195085	26.18%	2.542%
23	10.690	1225	1233	1239	rBB2	16517	26959	0.59%	0.057%
24	10.860	1255	1262	1278	rBV	1045517	1789759	39.20%	3.806%
25	11.007	1282	1287	1292	rVB2	8793	12562	0.28%	0.027%
26	11.137	1305	1309	1313	rBV	3225	4697	0.10%	0.010%
27	11.249	1320	1328	1343	rVB	939115	1591028	34.85%	3.384%
28	11.590	1382	1386	1395	rBV2	6140	10451	0.23%	0.022%
29	11.902	1434	1439	1444	rBV	5323	7983	0.17%	0.017%
30	12.460	1529	1534	1536	rBV	7476	10287	0.23%	0.022%
31	12.501	1536	1541	1546	rVB	34733	52738	1.16%	0.112%
32	12.807	1587	1593	1599	rBV	17666	26028	0.57%	0.055%
33	13.948	1782	1787	1791	rBV2	3997	5905	0.13%	0.013%
34	14.095	1807	1812	1816	rBV2	7612	9987	0.22%	0.021%

LSC Area Percent Report

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Misc :
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Instrument : BNA_N
ClientSampleId : BEEL3

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 >
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Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Title : SVOA CALIBRATION

35	14.296	1841	1846	1851	rBV2	4141	5458	0.12%	0.012%
36	14.419	1856	1867	1873	rBV	2012984	2760345	60.46%	5.870%
37	14.472	1873	1876	1880	rVB	6173	8115	0.18%	0.017%
38	14.731	1913	1920	1933	rBV	2252809	3417464	74.85%	7.268%
39	15.031	1958	1971	1980	rBV2	1321492	2091263	45.81%	4.448%
40	15.166	1989	1994	1997	rVV	19030	23775	0.52%	0.051%
41	15.219	1997	2003	2016	rVV	163783	266666	5.84%	0.567%
42	15.313	2016	2019	2023	rVB2	3448	4667	0.10%	0.010%
43	15.672	2071	2080	2085	rBV2	14860	26564	0.58%	0.056%
44	15.737	2085	2091	2097	rVV	597756	763946	16.73%	1.625%
45	15.801	2098	2102	2108	rVB2	21443	32833	0.72%	0.070%
46	16.013	2131	2138	2145	rBV	2818390	4021245	88.08%	8.552%
47	16.125	2151	2157	2170	rBV	712444	974674	21.35%	2.073%
48	16.248	2172	2178	2183	rVB2	30003	41130	0.90%	0.087%
49	16.337	2189	2193	2197	rBV	26046	33123	0.73%	0.070%
50	16.607	2231	2239	2240	rBV6	6256	11267	0.25%	0.024%
51	16.637	2240	2244	2249	rVV	128313	167677	3.67%	0.357%
52	16.689	2249	2253	2258	rVB5	3181	6009	0.13%	0.013%
53	17.542	2394	2398	2402	rVB	5571	6823	0.15%	0.015%
54	17.754	2427	2434	2441	rBV2	1632996	2314600	50.70%	4.922%
55	17.854	2444	2451	2461	rBV2	2956702	4246510	93.01%	9.031%
56	17.995	2471	2475	2478	rVB	3393	4982	0.11%	0.011%
57	18.584	2571	2575	2581	rBV	8136	10627	0.23%	0.023%
58	18.666	2585	2589	2593	rBV	9048	12151	0.27%	0.026%
59	18.860	2618	2622	2625	rBV2	3674	5535	0.12%	0.012%
60	18.895	2625	2628	2632	rVB2	10424	11876	0.26%	0.025%
61	19.113	2659	2665	2668	rVB5	8859	11680	0.26%	0.025%
62	19.354	2702	2706	2717	rBV	347225	448167	9.82%	0.953%
63	19.448	2718	2722	2727	rVV	20166	24114	0.53%	0.051%
64	19.748	2767	2773	2777	rBV	33250	45605	1.00%	0.097%
65	19.836	2783	2788	2795	rBV5	9343	16783	0.37%	0.036%
66	20.001	2810	2816	2820	rVB	24270	34860	0.76%	0.074%
67	20.113	2828	2835	2844	rBV	3171303	4565465	100.00%	9.709%
68	21.007	2985	2987	2992	rBV6	5848	6670	0.15%	0.014%
69	21.877	3129	3135	3141	rBV	1682245	2242336	49.12%	4.769%
70	22.448	3229	3232	3237	rVB	23462	27430	0.60%	0.058%
71	22.966	3314	3320	3335	rBV2	381612	669088	14.66%	1.423%

LSC Area Percent Report

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Instrument : BNA_N
ClientSampleId : BEEL3

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Title : SVOA CALIBRATION

72	23.513	3409	3413	3419	rVB2	93124	156855	3.44%	0.334%
73	24.142	3515	3520	3523	rBV	98832	184589	4.04%	0.393%
74	24.201	3523	3530	3542	rVB2	1631042	3376358	73.95%	7.181%
75	24.354	3548	3556	3565	rVB2	859033	1782473	39.04%	3.791%
76	24.866	3638	3643	3653	rVB	87177	184839	4.05%	0.393%
77	25.707	3780	3786	3796	rVB2	83306	197049	4.32%	0.419%

Sum of corrected areas: 47020965

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Instrument : BNA_N
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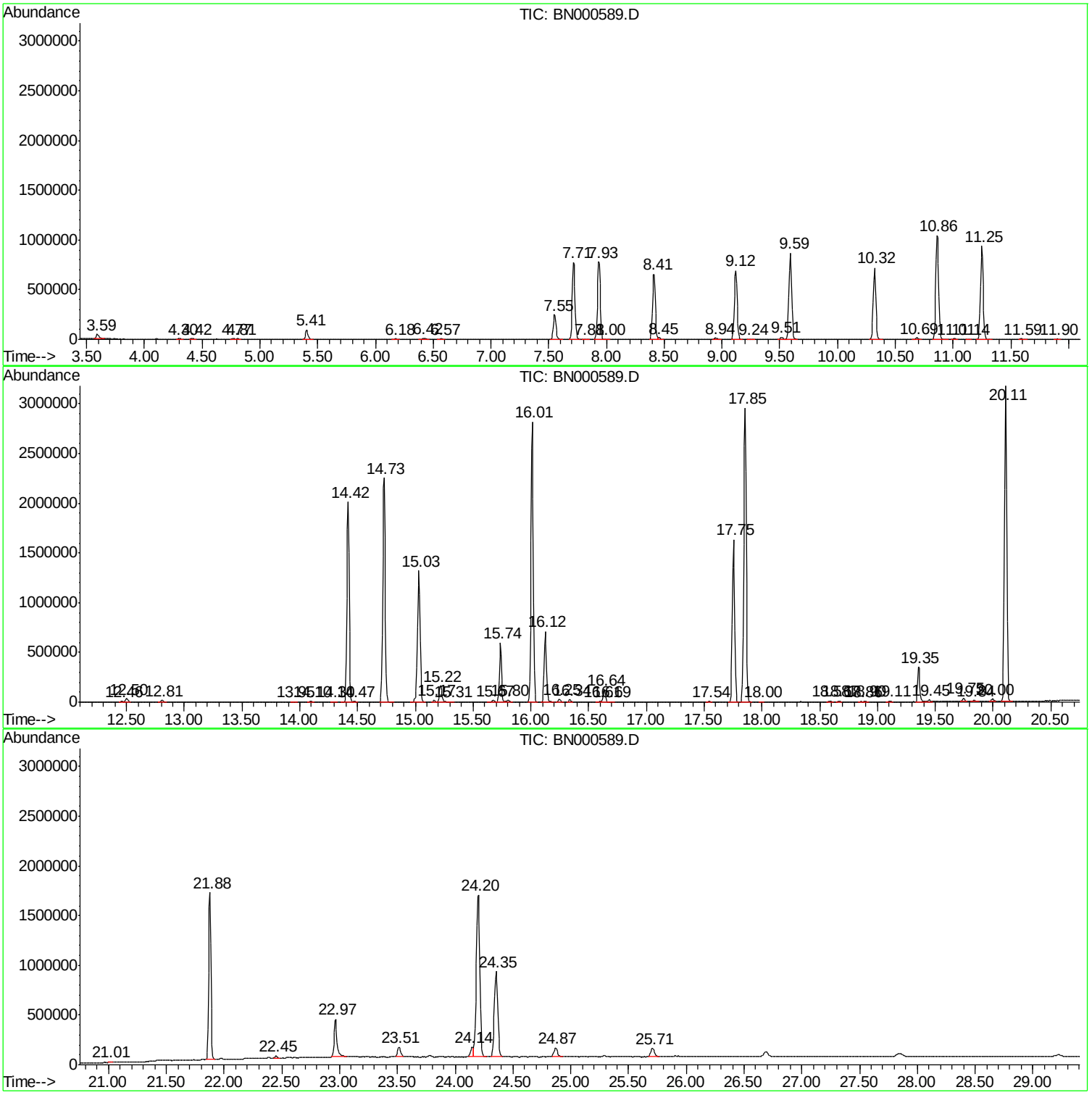
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN032318\
Data File : BN000589.D
Acq On : 23 Mar 2018 21:42
Operator : JU/SJ
Sample : J1986-22
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : BEEL3

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

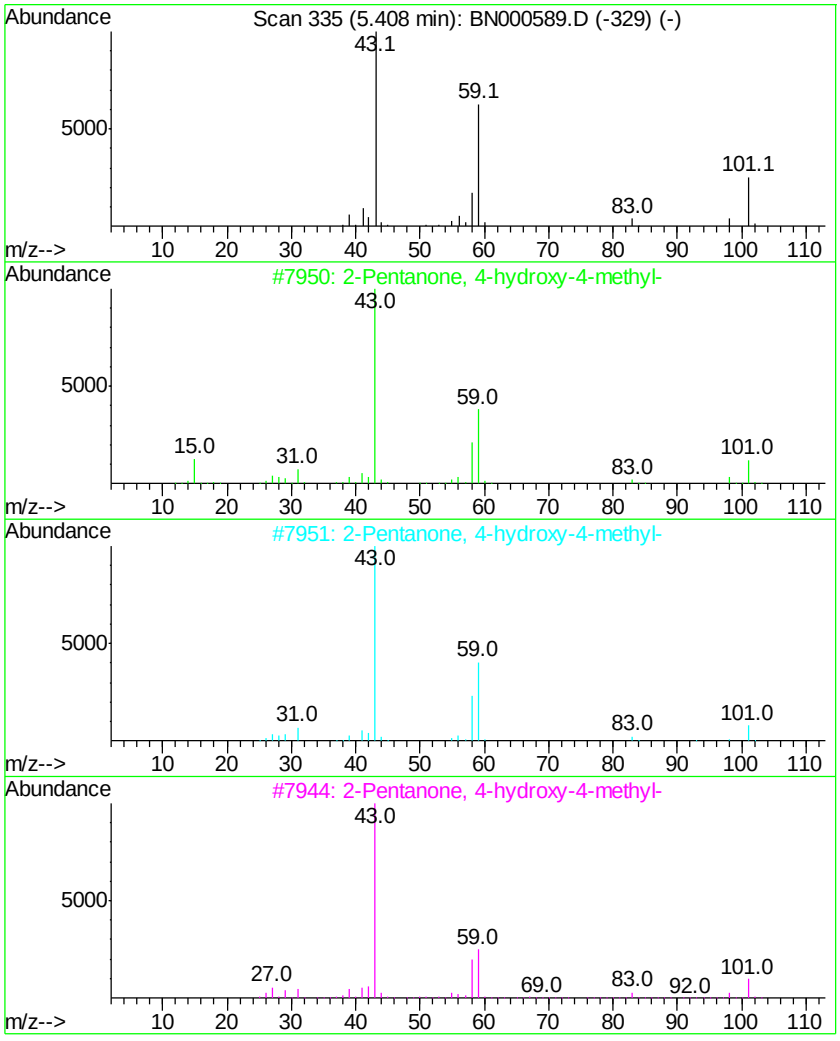
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

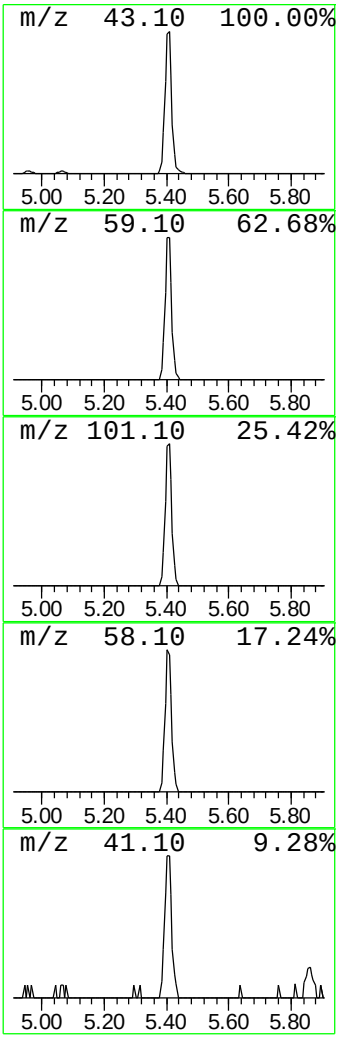
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.41	2.62 ng/ul	142218	1,4-Dichlorobenzene-d4	8.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Sample : J1986-22
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : BEEL3

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

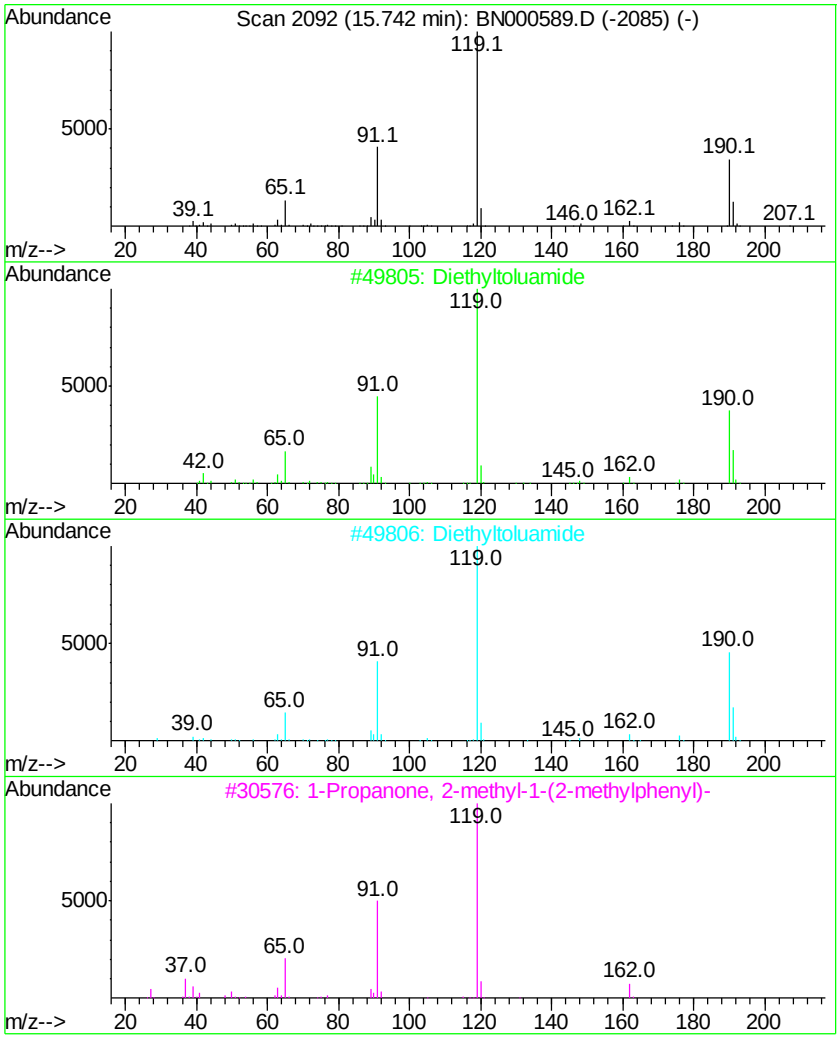
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

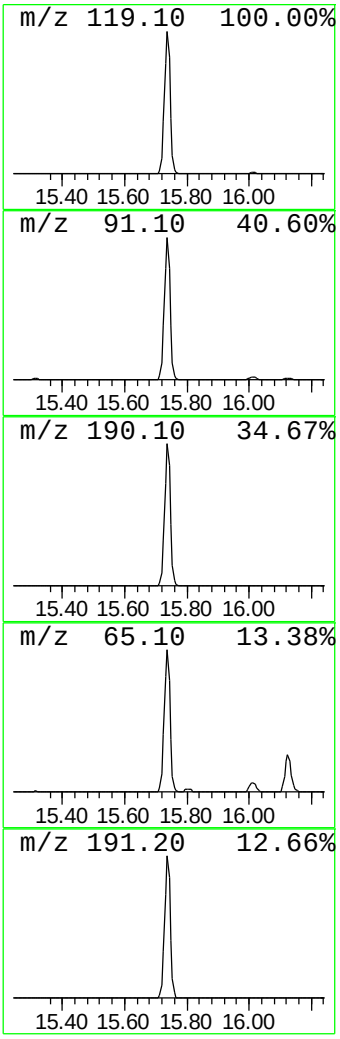
****

Peak Number 2 Diethyltoluamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	7.31 ng/ul	763946	Acenaphthene-d10	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	93
2	Diethyltoluamide	191	C12H17NO	000134-62-3	92
3	1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	74
4	N-[1-(Dimethylamino)-2,2,2-trich...	308	C12H15Cl3N2O	300814-41-9	72
5	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	72





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Instrument : BNA_N
ClientSampleId : BEEL3

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

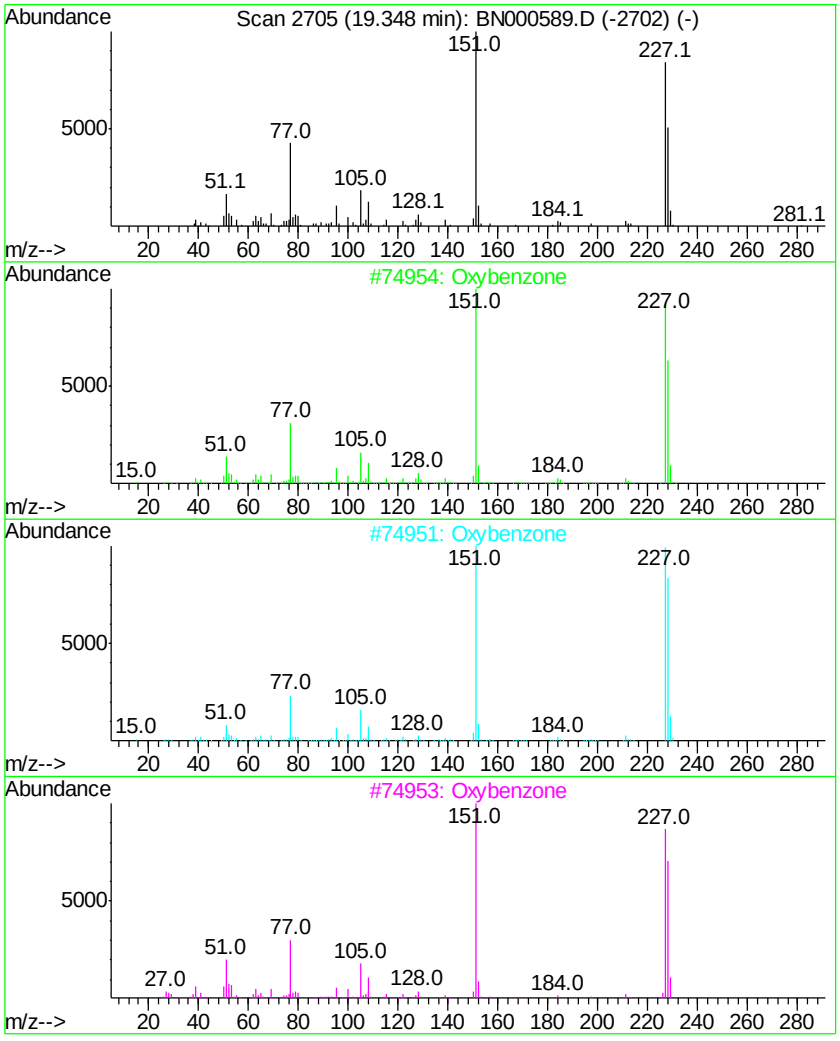
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

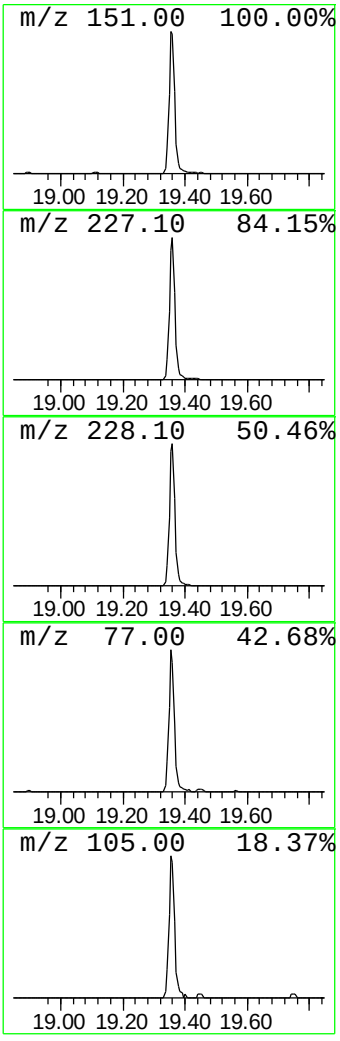
****

Peak Number 3 Oxybenzone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.87 ng/ul	448167	Phenanthrene-d10	17.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybenzone	228	C14H12O3	000131-57-7	98
2	Oxybenzone	228	C14H12O3	000131-57-7	97
3	Oxybenzone	228	C14H12O3	000131-57-7	97
4	Benzaldehyde, 3-methoxy-, oxime	151	C8H9NO2	038489-80-4	27
5	4-Amino-6-hydroxypyrazolo[3,4-d]...	151	C5H5N5O	005472-41-3	25





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Quant Title : SVOA CALIBRATION

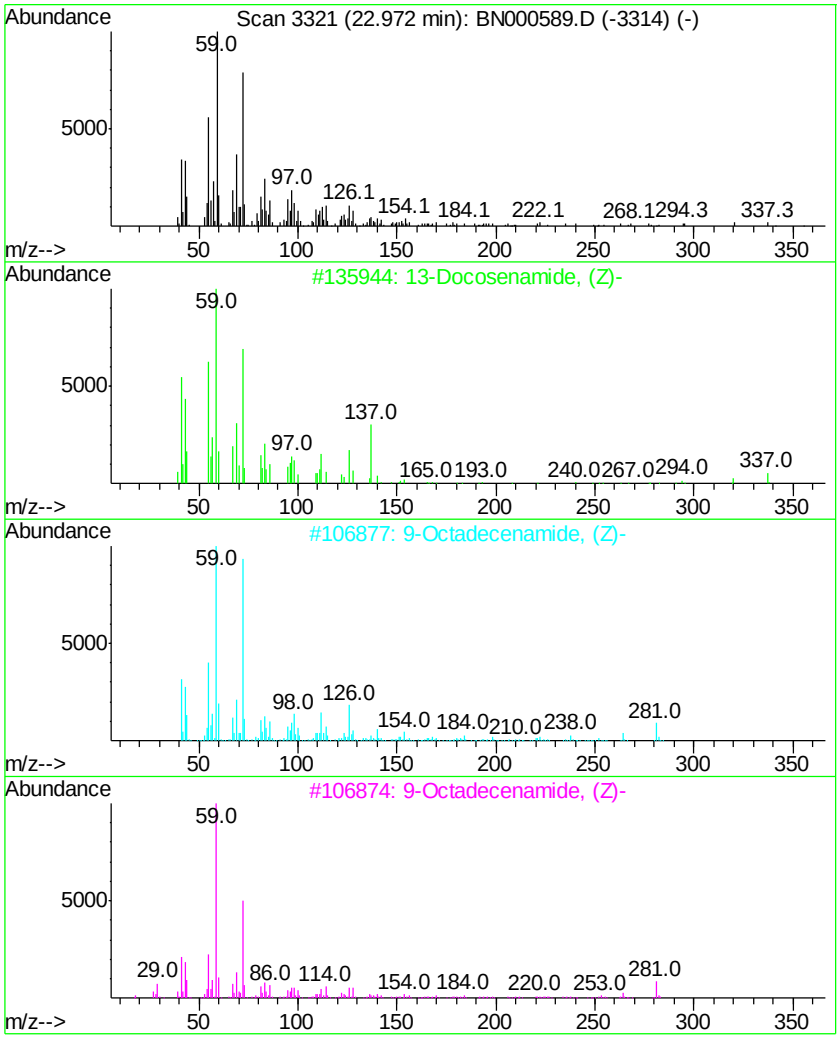
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

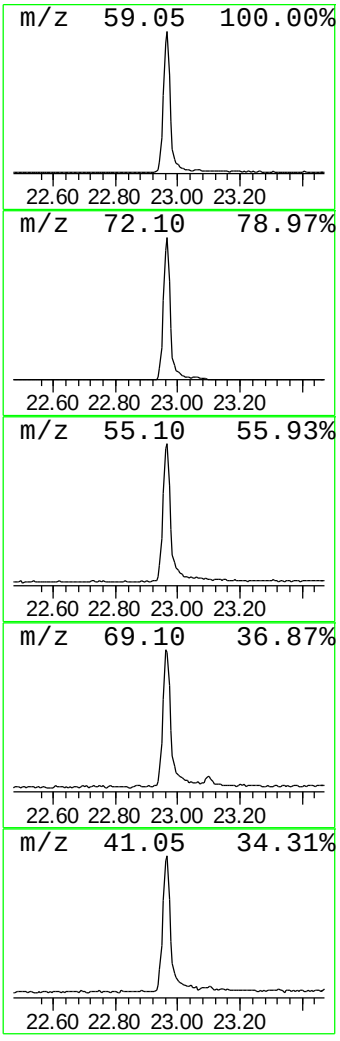
****

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.97	5.97 ng/ul	669088	Chrysene-d12	21.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	49
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	38
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	35





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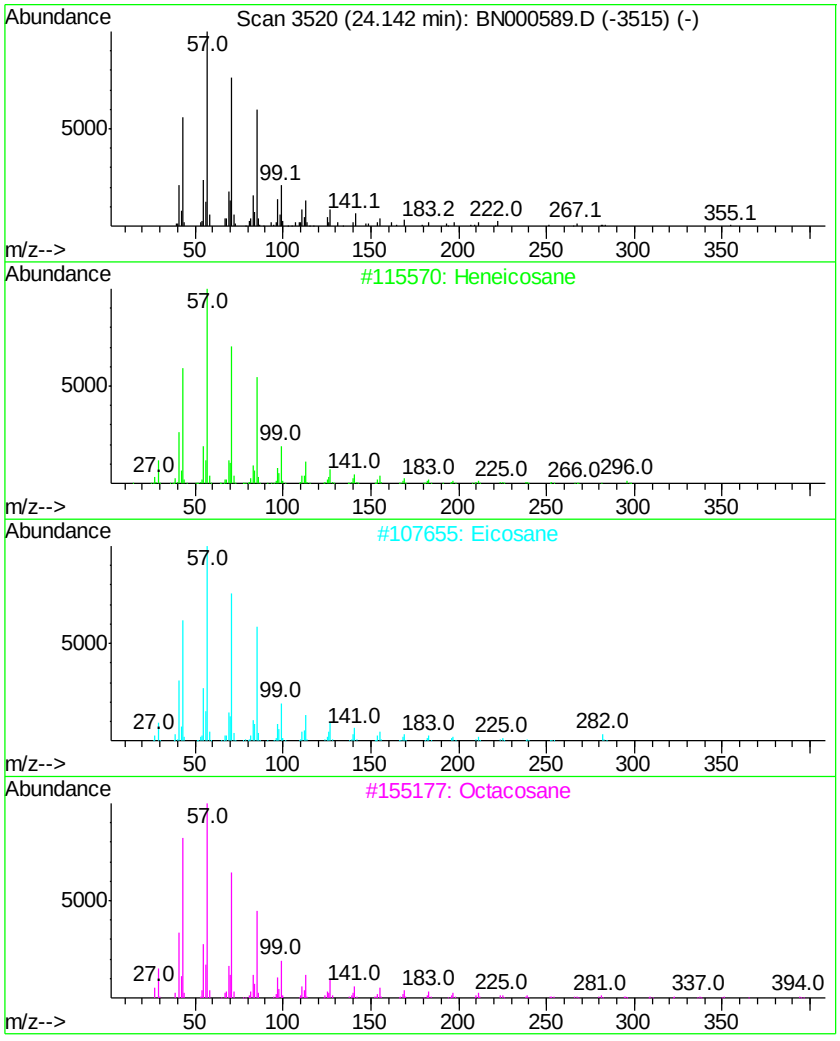
Quant Title : SVOA CALIBRATION

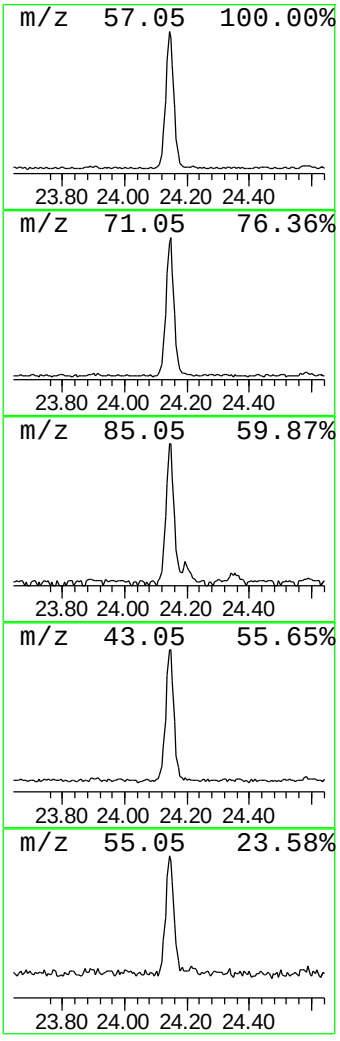
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	2.07 ng/ul	184589	Perylene-d12	24.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Octacosane	394	C28H58	000630-02-4	87





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Instrument : BNA_N
ClientSampleId : BEEL3

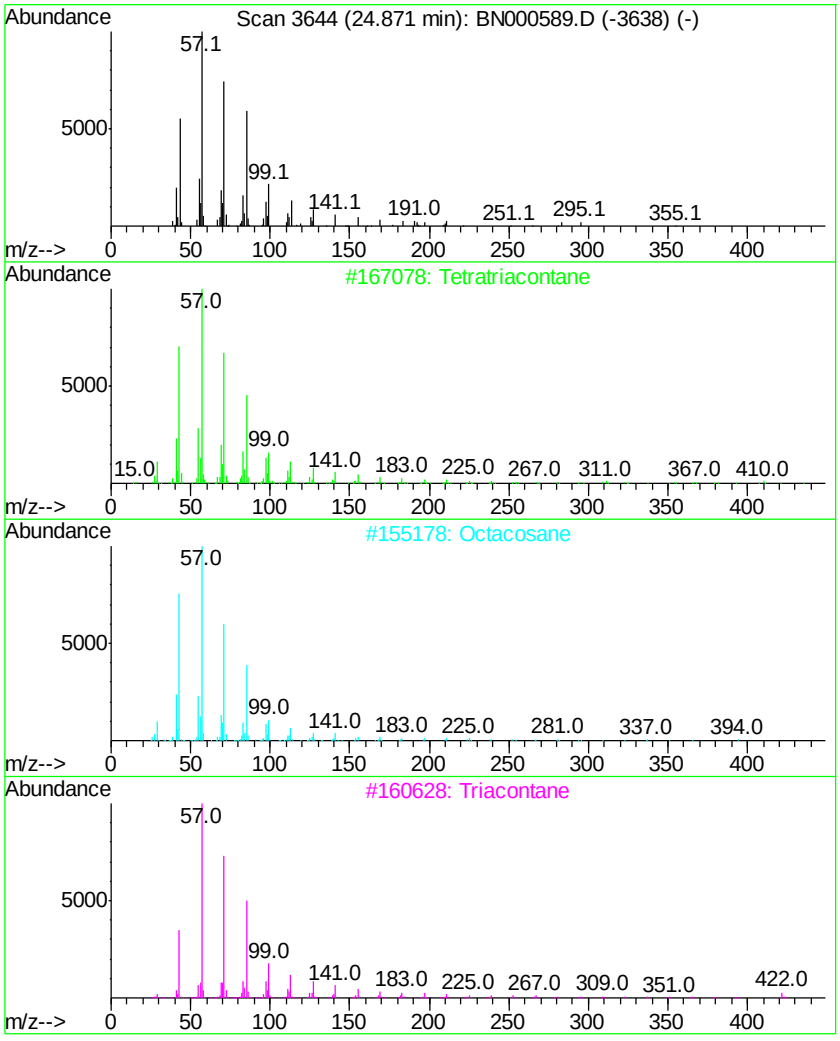
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

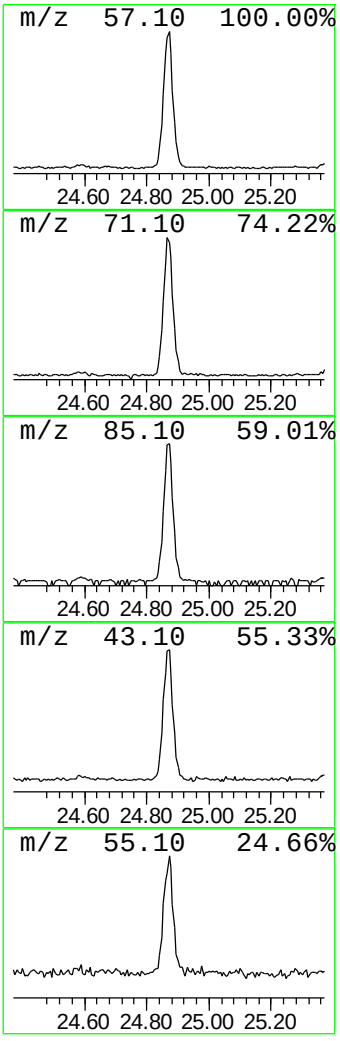
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.87	2.07 ng/ul	184839	Perylene-d12	24.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\HPCHEM1\BNA N\DATA\BN032318\
Data File : BN000589.D
Acq On : 23 Mar 2018 21:42
Operator : JU/SJ
Sample : J1986-22
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : BEEL3

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

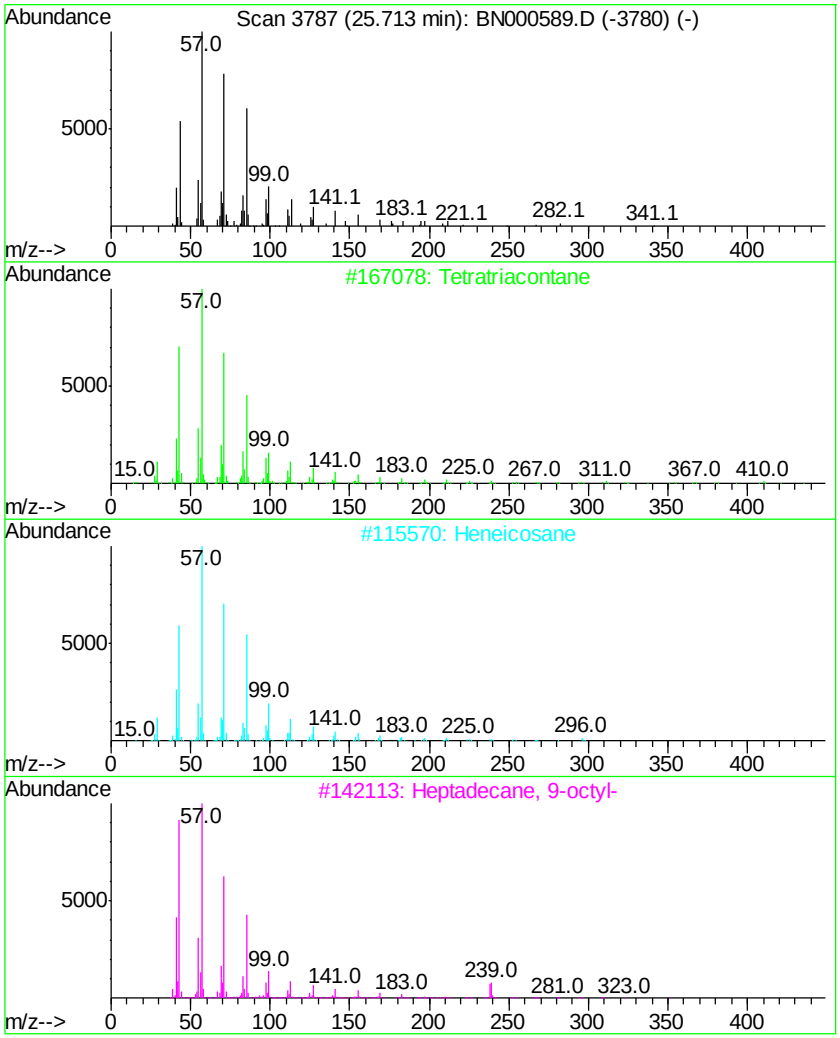
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

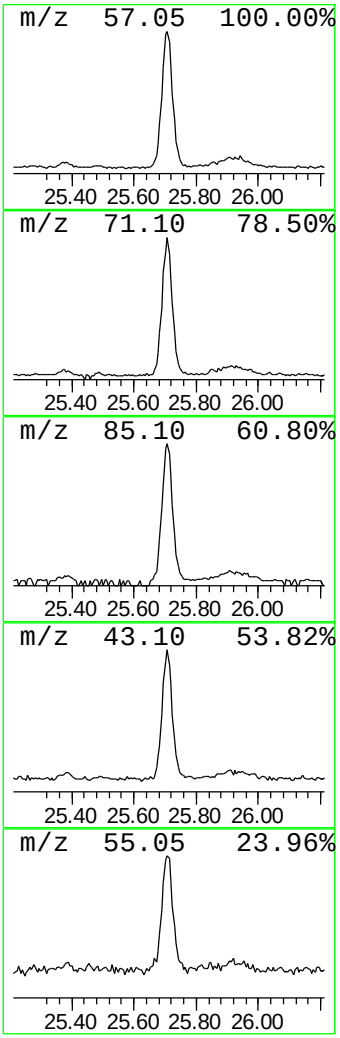
****

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.71	2.21 ng/ul	197049	Perylene-d12	24.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_N\DATA\BN032318\
Data File : BN000589.D
Acq On : 23 Mar 2018 21:42
Operator : JU/SJ
Sample : J1986-22
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : BEEL3

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN031918.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.41	2.6	ng/ul	142218	1	8.41	1087450	20.0
Diethyltoluamide	15.74	7.3	ng/ul	763946	3	15.03	2091260	20.0
Oxybenzone	19.35	3.9	ng/ul	448167	4	17.75	2314600	20.0
13-Docosenamide, ...	22.97	6.0	ng/ul	669088	5	21.88	2242340	20.0
(DEL) Alkane: Str...	24.14	2.1	ng/ul	184589	6	24.35	1782470	20.0
(DEL) Alkane: Str...	24.87	2.1	ng/ul	184839	6	24.35	1782470	20.0
(DEL) Alkane: Str...	25.71	2.2	ng/ul	197049	6	24.35	1782470	20.0