

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN052119\
 Data File : BN005835.D
 Acq On : 21 May 2019 21:18
 Operator : JU/SJ
 Sample : K2788-20
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 A51A2

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN051819MA.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	5.652	450	453	457	rBV	22923	33879	1.46%	0.188%
2	6.646	616	622	626	rBV2	36280	68210	2.95%	0.379%
3	6.734	634	637	639	rBV	25557	33878	1.46%	0.188%
4	6.769	639	643	656	rVB2	67406	155331	6.71%	0.862%
5	6.910	662	667	676	rVB	164792	282086	12.19%	1.566%
6	7.105	695	700	713	rVB	206142	386888	16.72%	2.147%
7	7.563	773	778	786	rBV	197858	335590	14.51%	1.863%
8	7.634	786	790	797	rVB	26047	43305	1.87%	0.240%
9	7.822	819	822	827	rBV3	18191	29220	1.26%	0.162%
10	8.281	895	900	913	rVB	161994	333164	14.40%	1.849%
11	8.652	958	963	968	rBV	79470	141075	6.10%	0.783%
12	8.710	968	973	982	rVB	224557	421774	18.23%	2.341%
13	8.881	999	1002	1012	rVB4	22057	39932	1.73%	0.222%
14	9.428	1089	1095	1106	rBV2	189567	366774	15.85%	2.036%
15	9.599	1119	1124	1131	rVB4	17868	42343	1.83%	0.235%
16	9.816	1157	1161	1162	rBV2	21809	27104	1.17%	0.150%
17	9.981	1183	1189	1204	rBV	182562	506906	21.91%	2.814%
18	10.322	1241	1247	1254	rBV	279776	466956	20.18%	2.592%
19	11.116	1379	1382	1387	rVB5	7232	9489	0.41%	0.053%
20	12.540	1619	1624	1630	rBV3	21868	36227	1.57%	0.201%
21	12.798	1663	1668	1675	rBV	38048	59303	2.56%	0.329%
22	13.140	1721	1726	1746	rVB3	79679	227775	9.85%	1.264%
23	13.622	1802	1808	1822	rVB	550932	872492	37.71%	4.843%
24	13.892	1847	1854	1868	rVB	660133	993593	42.95%	5.515%
25	14.087	1883	1887	1889	rBV2	3314	4088	0.18%	0.023%
26	14.122	1889	1893	1898	rVV3	5879	12035	0.52%	0.067%
27	14.198	1900	1906	1915	rVB2	439431	668772	28.91%	3.712%
28	14.292	1919	1922	1927	rVB2	2399	2970	0.13%	0.016%
29	14.510	1954	1959	1968	rBV5	15564	51437	2.22%	0.285%
30	15.016	2041	2045	2048	rVV	13622	18349	0.79%	0.102%
31	15.051	2048	2051	2056	rVB	15899	20320	0.88%	0.113%
32	15.204	2071	2077	2088	rBV	813471	1283381	55.47%	7.123%
33	15.381	2102	2107	2116	rVV	126941	250090	10.81%	1.388%
34	15.451	2116	2119	2130	rVB5	11790	19583	0.85%	0.109%

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35	15.586	2136	2142	2149	rBV2	6067	7885	0.34%	0.044%
36	15.998	2209	2212	2216	rVB3	2725	3492	0.15%	0.019%
37	16.963	2369	2376	2386	rBV	617619	870773	37.64%	4.833%
38	17.063	2386	2393	2408	rVB2	879305	1411219	61.00%	7.833%
39	17.251	2423	2425	2426	rBV	2702	2516	0.11%	0.014%
40	17.263	2426	2427	2432	rVB	3035	2380	0.10%	0.013%
41	17.633	2485	2490	2497	rBV	316907	376102	16.26%	2.088%
42	17.886	2530	2533	2535	rBV3	1868	2735	0.12%	0.015%
43	17.951	2538	2544	2550	rBV3	4994	9785	0.42%	0.054%
44	18.451	2623	2629	2637	rVB2	38478	49076	2.12%	0.272%
45	19.016	2719	2725	2729	rBV2	8772	12676	0.55%	0.070%
46	19.239	2759	2763	2764	rBV2	1791	2381	0.10%	0.013%
47	19.263	2764	2767	2773	rVV2	7505	10583	0.46%	0.059%
48	19.375	2780	2786	2804	rVV	1229933	1845468	79.77%	10.243%
49	20.551	2984	2986	2989	rBV4	2907	2575	0.11%	0.014%
50	20.669	3004	3006	3008	rBV3	2834	2430	0.11%	0.013%
51	20.910	3045	3047	3050	rBV4	5312	6294	0.27%	0.035%
52	21.198	3091	3096	3108	rBV	805496	1204116	52.05%	6.683%
53	21.357	3121	3123	3124	rBV2	7353	4611	0.20%	0.026%
54	22.233	3269	3272	3276	rBV4	34513	44045	1.90%	0.244%
55	22.727	3353	3356	3360	rVB	36850	46263	2.00%	0.257%
56	23.257	3439	3446	3459	rBV	1240443	2313490	100.00%	12.841%
57	23.398	3463	3470	3484	rVB	631446	1355530	58.59%	7.524%
58	23.892	3550	3554	3560	rVB3	54504	96414	4.17%	0.535%
59	24.604	3672	3675	3683	rVB6	45388	89370	3.86%	0.496%

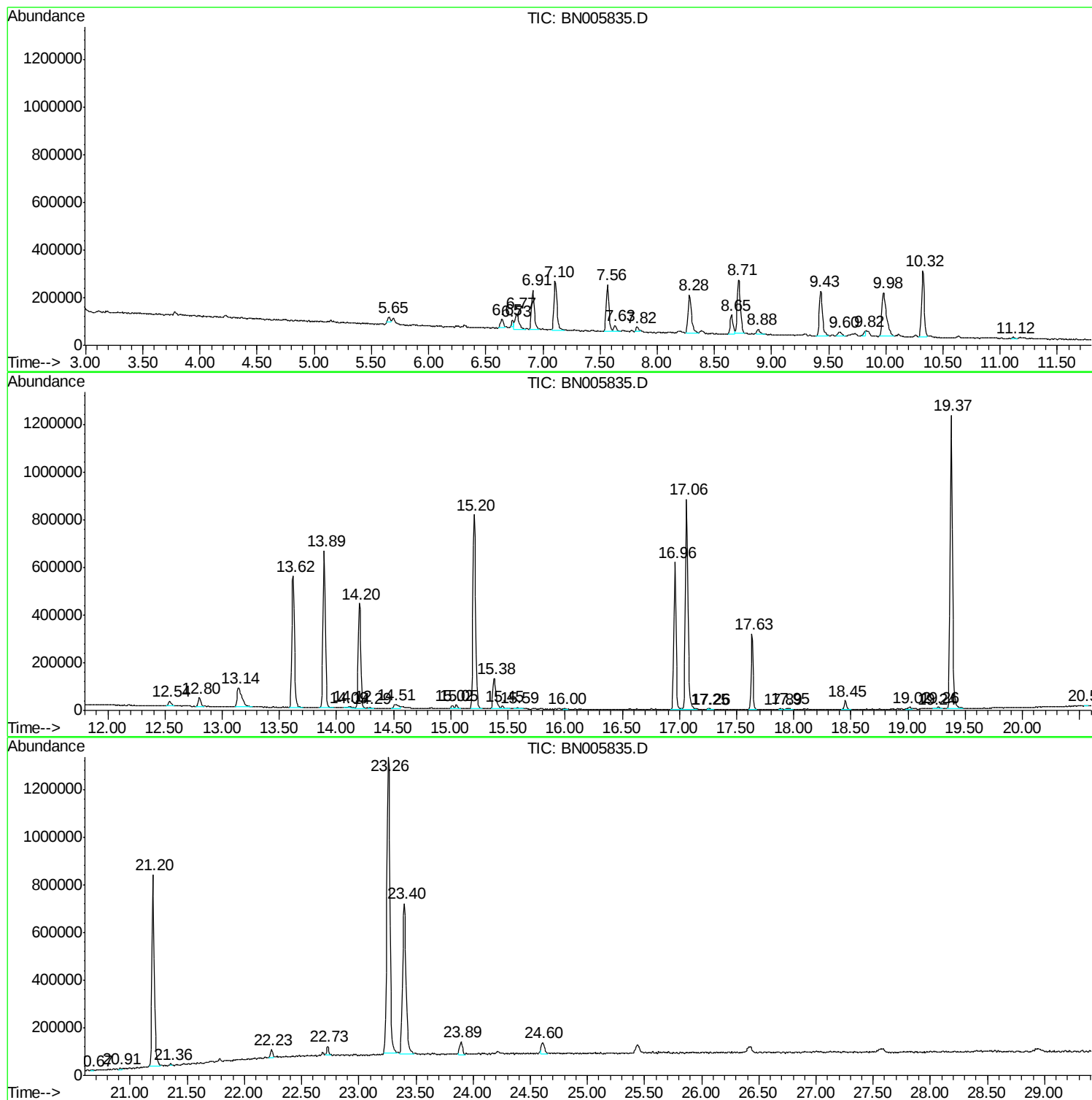
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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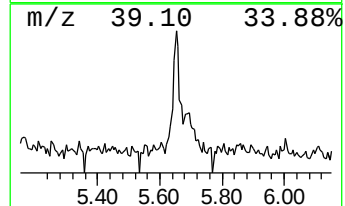
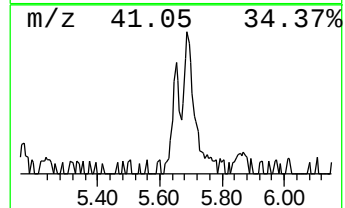
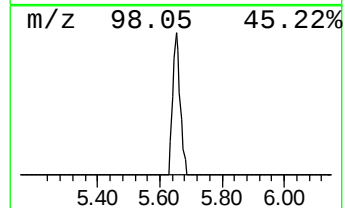
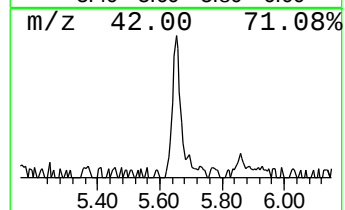
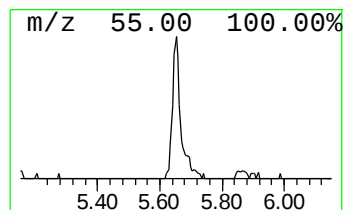
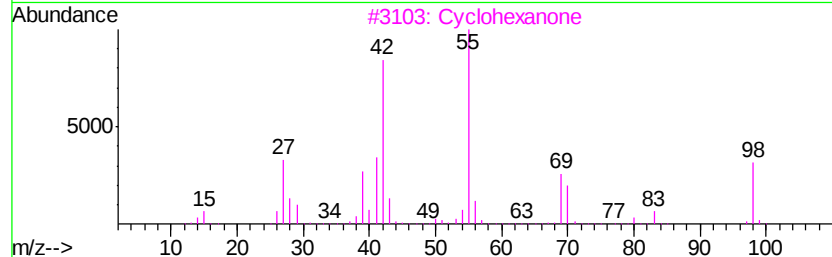
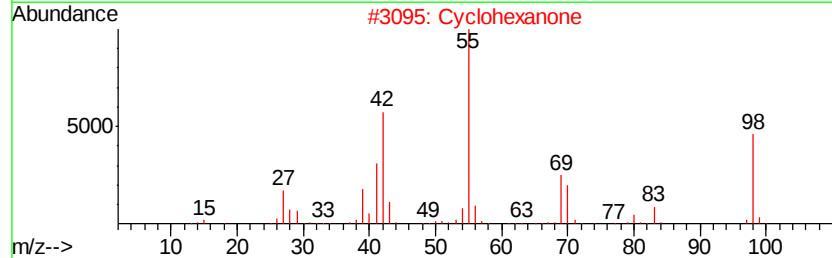
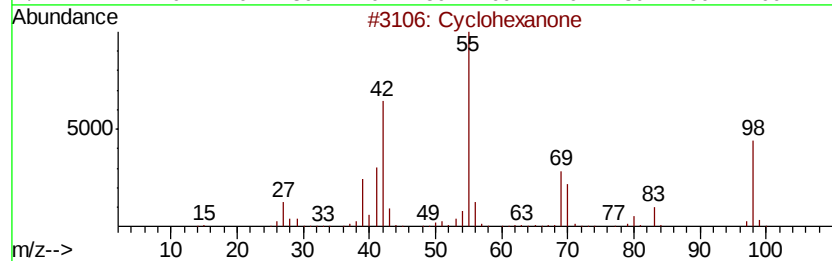
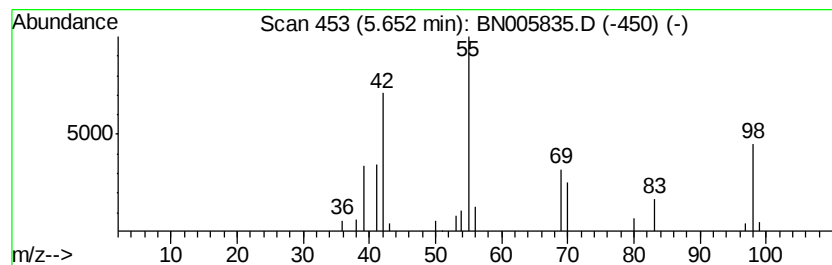
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cyclohexanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	2.02 ng/ul	33879	1,4-Dichlorobenzene-d4	7.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	91
2			Cyclohexanone	98	C6H10O	000108-94-1	91
3			Cyclohexanone	98	C6H10O	000108-94-1	91
4			Cyclohexanone	98	C6H10O	000108-94-1	90
5			Cyclohexanone	98	C6H10O	000108-94-1	78



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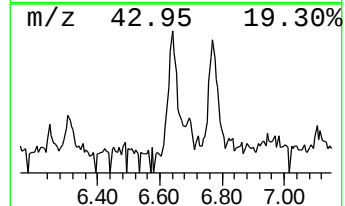
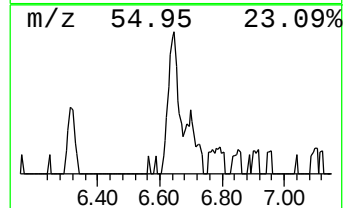
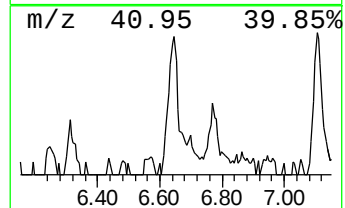
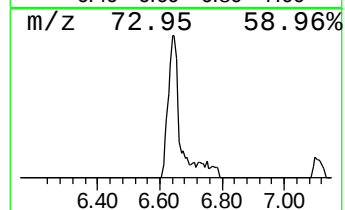
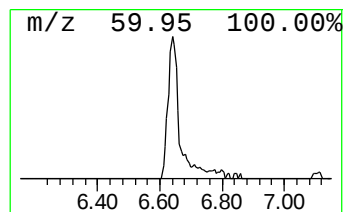
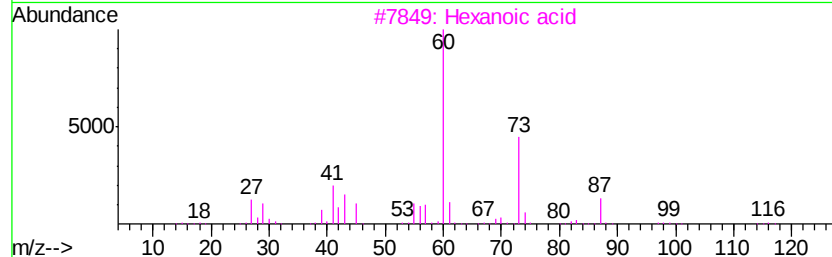
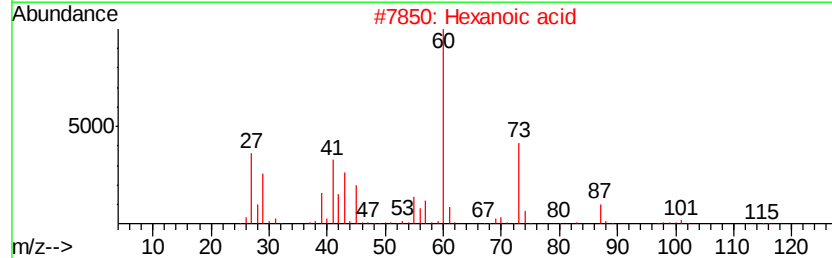
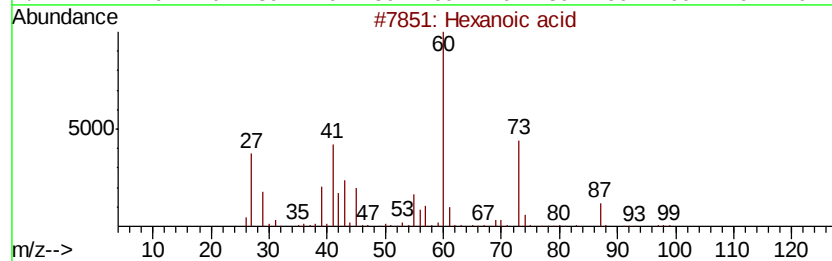
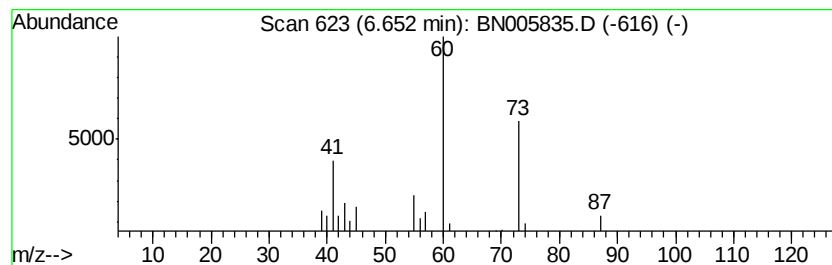
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 Hexanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	4.07 ng/ul	68210	1,4-Dichlorobenzene-d4	7.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	83
2			Hexanoic acid	116	C6H12O2	000142-62-1	78
3			Hexanoic acid	116	C6H12O2	000142-62-1	72
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



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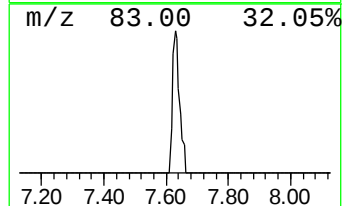
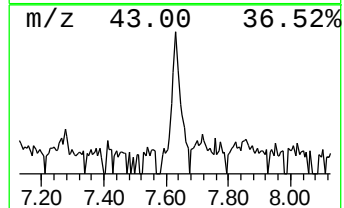
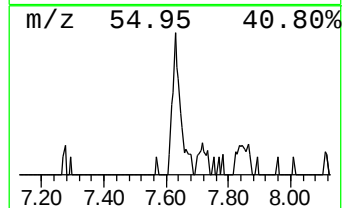
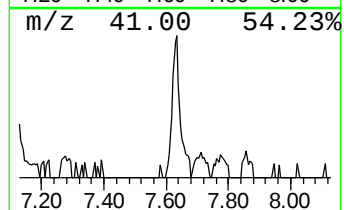
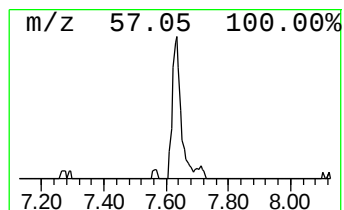
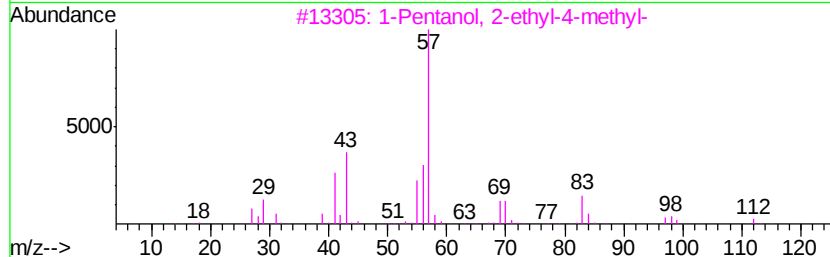
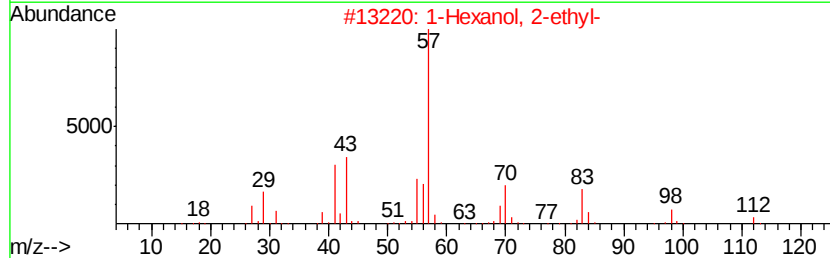
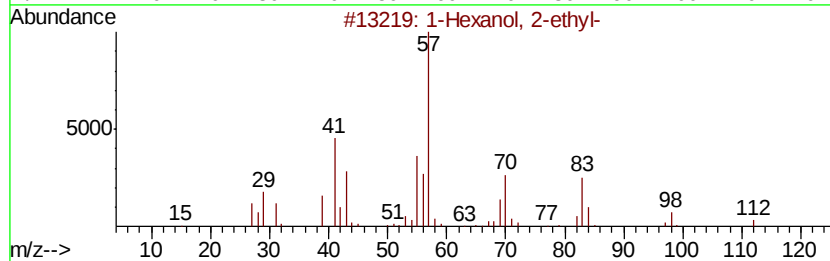
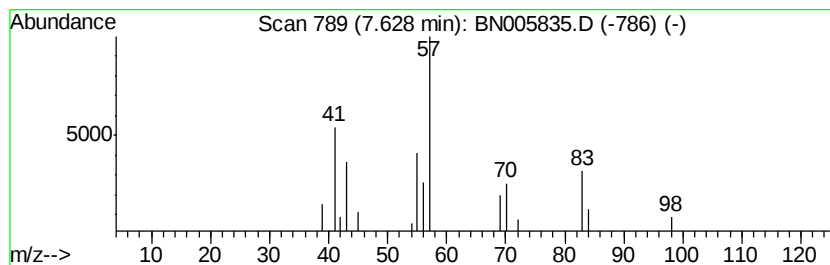
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	2.58 ng/ul	43305	1,4-Dichlorobenzene-d4	7.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50
5			2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	47



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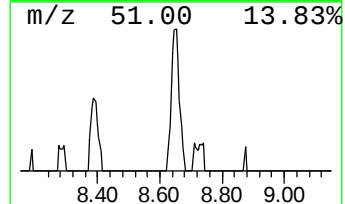
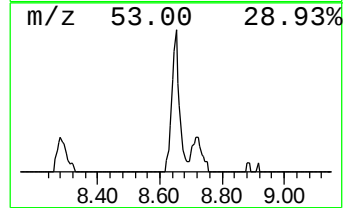
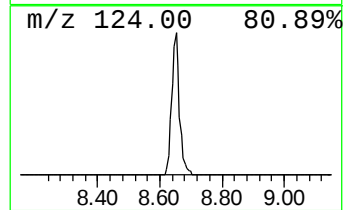
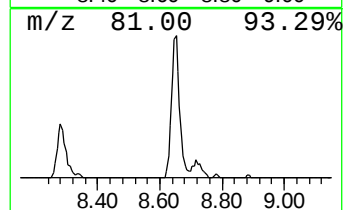
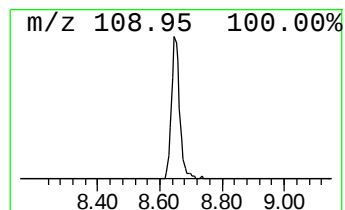
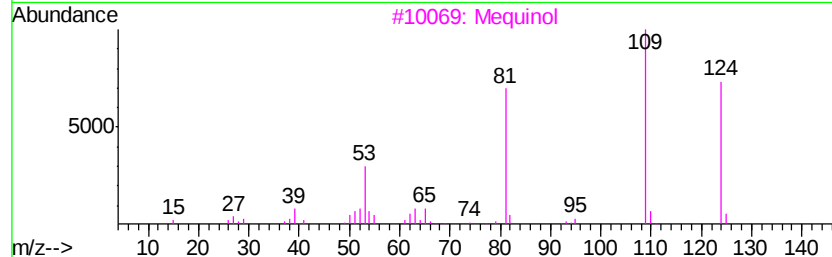
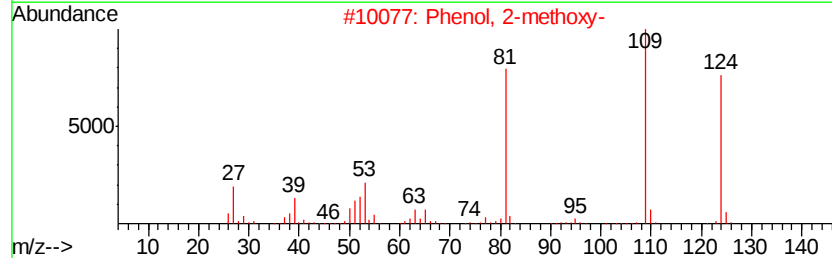
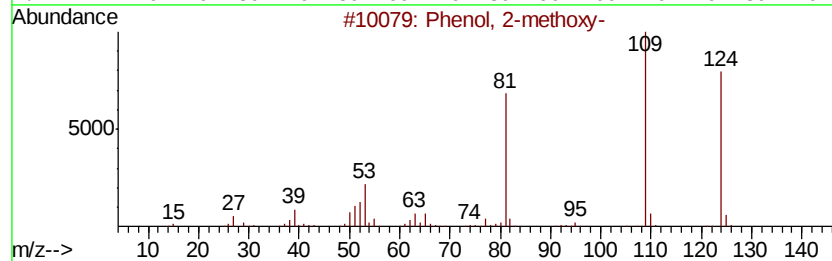
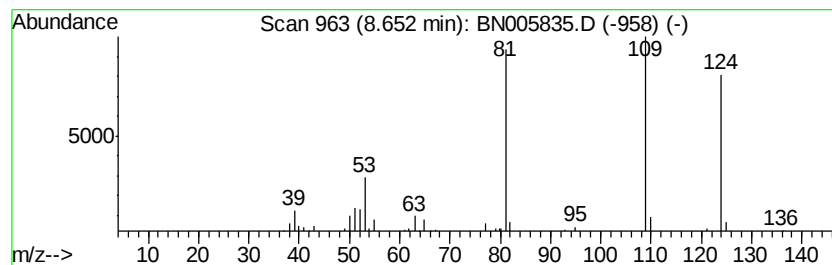
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 2-methoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	8.41 ng/ul	141075	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
2		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
3		Mequinol	124	C7H8O2	000150-76-5	91
4		Mequinol	124	C7H8O2	000150-76-5	90
5		2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	90



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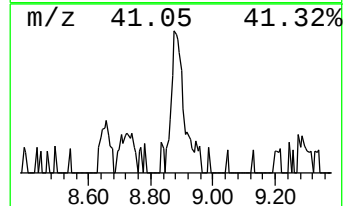
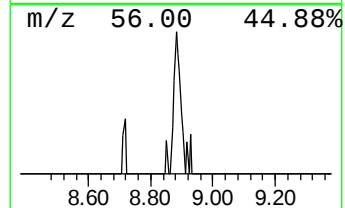
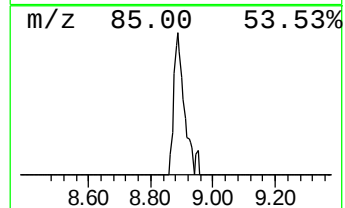
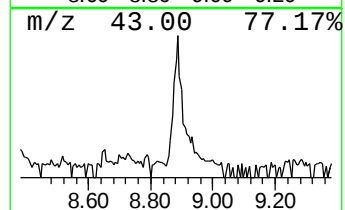
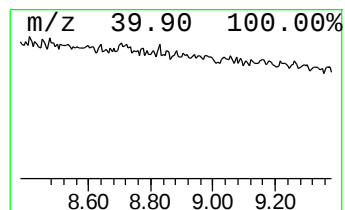
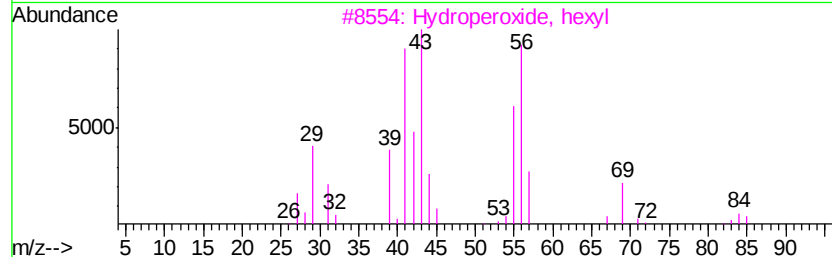
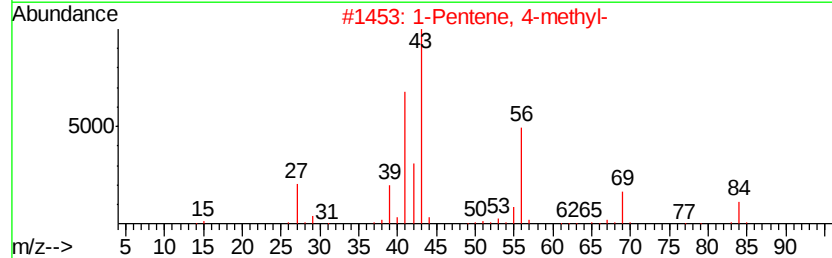
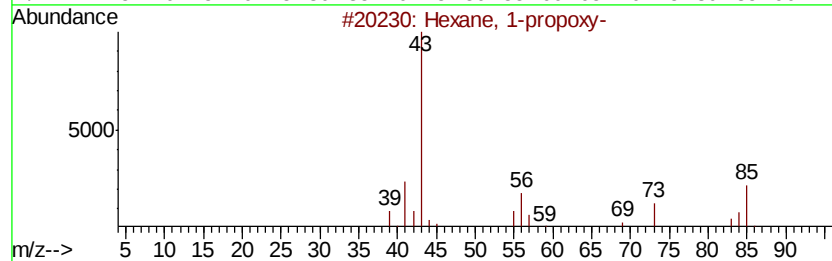
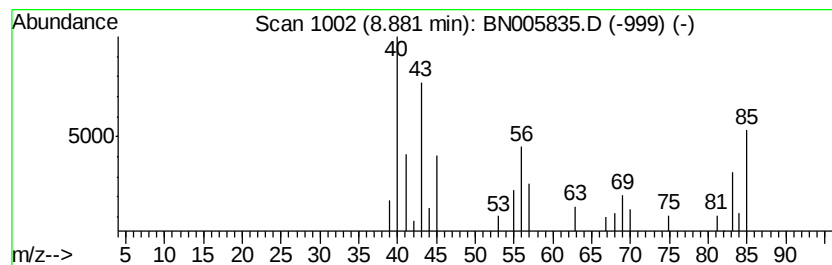
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	2.38 ng/ul	39932	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 1-propoxy-	144	C9H20O	053685-78-2	17
2		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	9
3		Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	9
4		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	9
5		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN052119\
Data File : BN005835.D
Acq On : 21 May 2019 21:18
Operator : JU/SJ
Sample : K2788-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A51A2

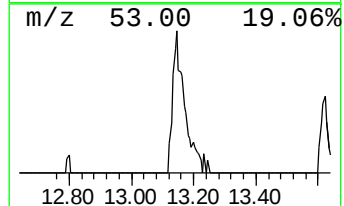
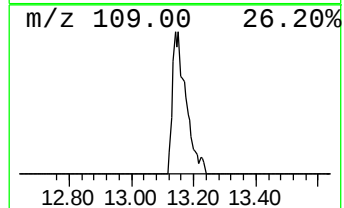
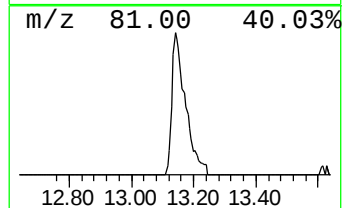
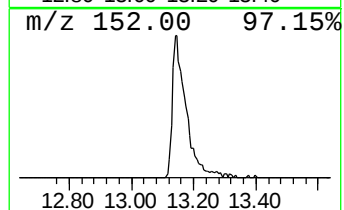
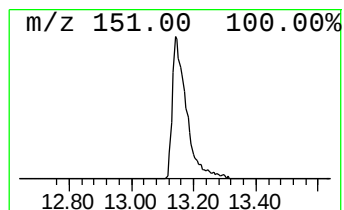
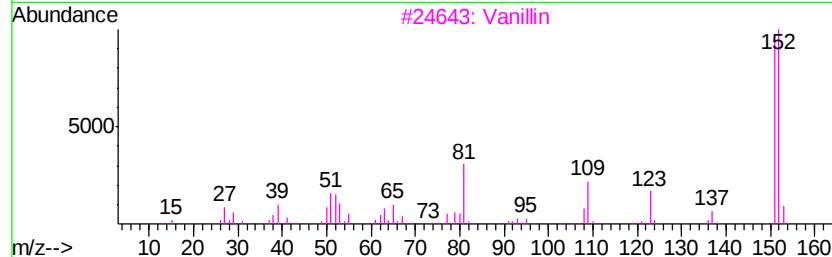
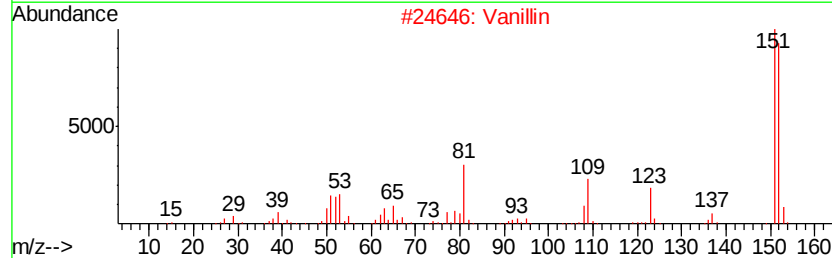
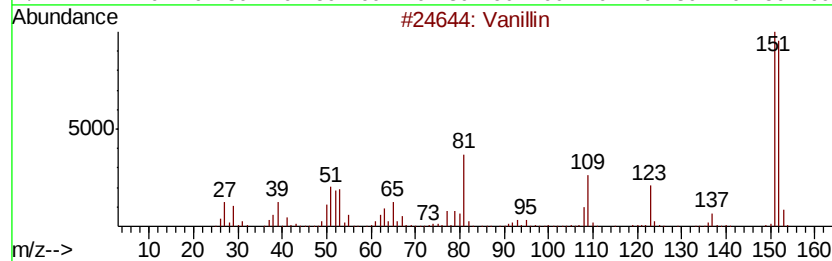
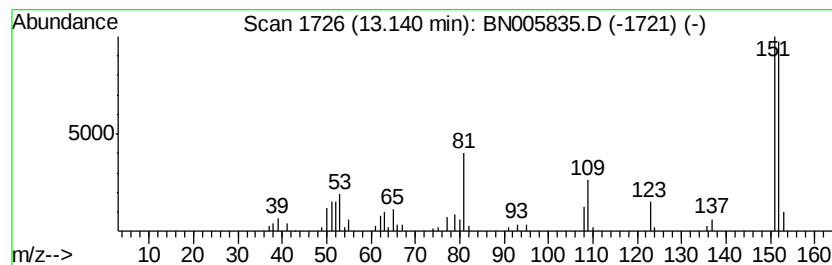
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Vanillin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	6.81 ng/ul	227775	Acenaphthene-d10	14.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin		152	C8H8O3	000121-33-5	98
2	Vanillin		152	C8H8O3	000121-33-5	96
3	Vanillin		152	C8H8O3	000121-33-5	96
4	Benzaldehyde, 3-hydroxy-4-methoxy-		152	C8H8O3	000621-59-0	96
5	Vanillin		152	C8H8O3	000121-33-5	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN052119\
Data File : BN005835.D
Acq On : 21 May 2019 21:18
Operator : JU/SJ
Sample : K2788-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A51A2

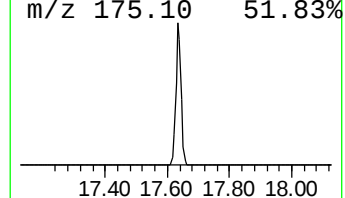
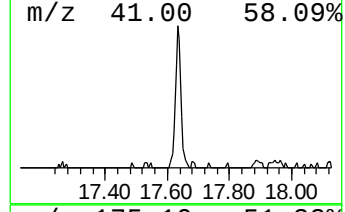
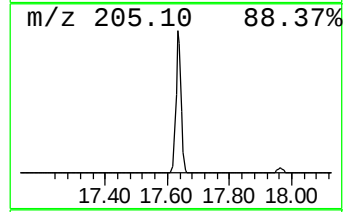
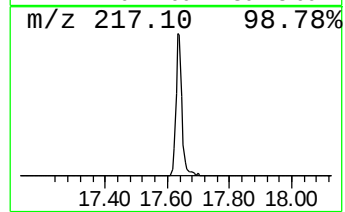
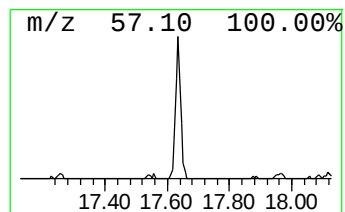
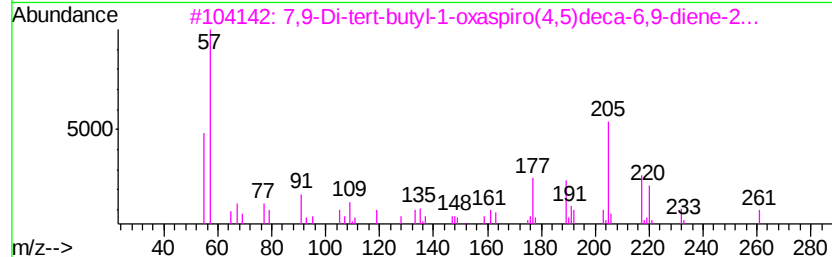
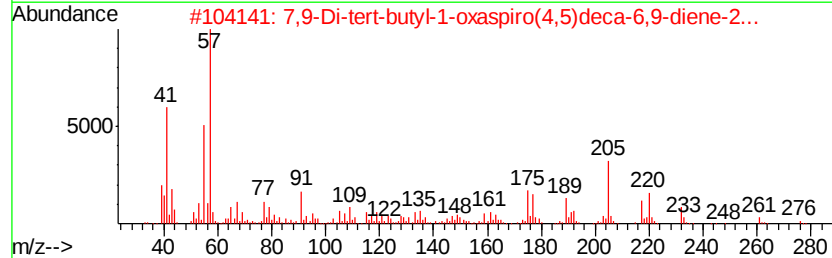
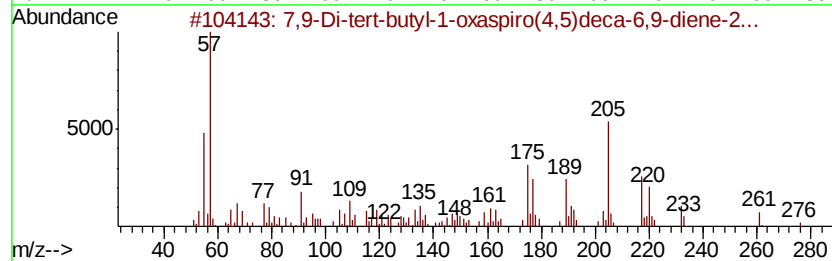
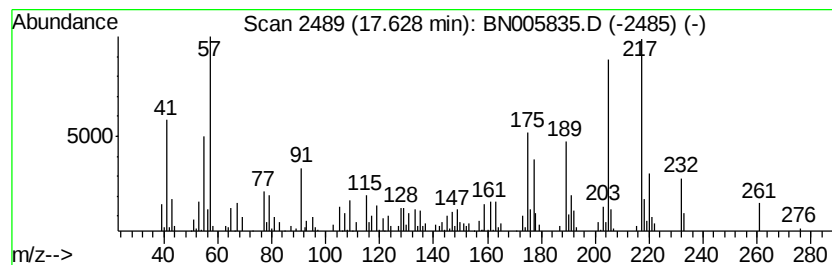
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	8.64 ng/ul	376102	Phenanthrene-d10	16.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	95		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	91		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	58		
4	Ethanone, 1-(5,6,7,8-tetrahydro-2H-chromen-2-yl)-	220	C14H20O2	071596-88-8	38		
5	4-Amino-7-diethylamino-chromen-2-one	232	C13H16N2O2	107995-76-6	38		



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Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN051819MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone	5.65	2.0	ng/ul	33879	1	7.56	335590	20.0
Hexanoic acid	6.65	4.1	ng/ul	68210	1	7.56	335590	20.0
1-Hexanol, 2-ethyl-	7.63	2.6	ng/ul	43305	1	7.56	335590	20.0
Phenol, 2-methoxy-	8.65	8.4	ng/ul	141075	1	7.56	335590	20.0
unknown-01	8.88	2.4	ng/ul	39932	1	7.56	335590	20.0
Vanillin	13.14	6.8	ng/ul	227775	3	14.20	668772	20.0
7,9-Di-tert-butyl...	17.63	8.6	ng/ul	376102	4	16.96	870773	20.0