

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
 Data File : BN029887.D
 Acq On : 21 Feb 2024 13:16
 Operator : MA/JU
 Sample : P1456-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BHA08

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_N\Methods\SFAM-EPA-BN020724.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN029887.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	36	39	44	rBV	48313	61110	1.11%	0.108%
2	3.728	106	109	129	rBV	274277	520405	9.45%	0.923%
3	4.046	161	163	169	rVB	13595	17357	0.32%	0.031%
4	4.417	224	226	237	rVB8	10680	21949	0.40%	0.039%
5	4.905	305	309	314	rBV4	8098	13826	0.25%	0.025%
6	5.411	391	395	401	rVB	15410	24377	0.44%	0.043%
7	5.517	409	413	418	rVB2	14266	21574	0.39%	0.038%
8	5.952	484	487	497	rVB2	13770	25210	0.46%	0.045%
9	6.864	635	642	647	rBV	28498	55007	1.00%	0.098%
10	7.028	662	670	682	rVB	264654	502240	9.12%	0.891%
11	7.205	693	700	710	rBV	839702	1319377	23.95%	2.341%
12	7.387	724	731	740	rBV	850010	1332170	24.19%	2.364%
13	7.858	804	811	818	rBV	648808	1012336	18.38%	1.796%
14	7.922	818	822	830	rVB	67049	110986	2.02%	0.197%
15	8.111	850	854	858	rBV	26316	45208	0.82%	0.080%
16	8.146	858	860	865	rVB2	13055	17719	0.32%	0.031%
17	8.428	902	908	913	rVV6	10269	20510	0.37%	0.036%
18	8.487	913	918	926	rBV	39376	67101	1.22%	0.119%
19	8.569	926	932	943	rVV	657467	1060544	19.26%	1.882%
20	8.693	948	953	962	rVB	35510	63821	1.16%	0.113%
21	8.958	990	998	1004	rBV	645507	1039342	18.87%	1.844%
22	9.028	1004	1010	1016	rVV	995959	1641190	29.80%	2.912%
23	9.075	1016	1018	1024	rVV	24942	43785	0.79%	0.078%
24	9.134	1026	1028	1031	rVV4	10226	13331	0.24%	0.024%
25	9.199	1034	1039	1045	rVB8	17854	38637	0.70%	0.069%
26	9.410	1071	1075	1080	rBV3	10444	17371	0.32%	0.031%
27	9.746	1123	1132	1145	rBV	751183	1256617	22.81%	2.230%
28	9.899	1153	1158	1166	rVB7	10592	25064	0.46%	0.044%
29	9.981	1166	1172	1181	rVB4	18362	36061	0.65%	0.064%
30	10.275	1214	1222	1233	rBV	1055082	1812987	32.92%	3.217%
31	10.452	1245	1252	1261	rVB9	13771	33456	0.61%	0.059%
32	10.569	1266	1272	1280	rVB3	64841	122035	2.22%	0.217%
33	10.657	1280	1287	1294	rBV	810915	1371304	24.90%	2.433%
34	10.716	1294	1297	1303	rVB2	41105	68097	1.24%	0.121%
35	10.805	1303	1312	1327	rBV	902272	1635755	29.70%	2.903%
36	11.040	1345	1352	1365	rVB4	12035	30752	0.56%	0.055%

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
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37	11.210	1375	1381	1385	rBV	13077	24352	0.44%	0.043%
38	11.263	1387	1390	1394	rVV2	13141	21572	0.39%	0.038%
39	11.316	1394	1399	1408	rVB	46804	84403	1.53%	0.150%
40	11.416	1410	1416	1419	rBV7	9154	18318	0.33%	0.033%

41	11.457	1419	1423	1429	rVV3	20619	31136	0.57%	0.055%
42	11.569	1437	1442	1451	rVB5	7413	14589	0.26%	0.026%
43	11.652	1451	1456	1467	rBV5	13581	30782	0.56%	0.055%
44	11.834	1481	1487	1491	rBV	31392	52037	0.94%	0.092%
45	11.869	1491	1493	1497	rVB4	9458	12451	0.23%	0.022%

46	11.952	1500	1507	1521	rBV	162482	287890	5.23%	0.511%
47	12.246	1548	1557	1563	rBV	23904	49513	0.90%	0.088%
48	12.516	1598	1603	1607	rVB	17034	23885	0.43%	0.042%
49	12.716	1629	1637	1641	rBV5	18456	33455	0.61%	0.059%
50	12.781	1641	1648	1657	rVV	80990	176374	3.20%	0.313%

51	12.869	1659	1663	1670	rVB7	12835	25239	0.46%	0.045%
52	12.975	1677	1681	1686	rBV	21229	27832	0.51%	0.049%
53	13.116	1700	1705	1711	rBV	32074	47965	0.87%	0.085%
54	13.263	1725	1730	1734	rVB7	8751	14882	0.27%	0.026%
55	13.351	1740	1745	1750	rVB	22962	35351	0.64%	0.063%

56	13.434	1750	1759	1775	rBV	1280249	2009439	36.48%	3.566%
57	13.928	1836	1843	1849	rBV	1954756	2733398	49.63%	4.851%
58	14.034	1857	1861	1867	rVB6	10177	15232	0.28%	0.027%
59	14.198	1878	1889	1896	rBV2	2167450	3294998	59.82%	5.847%
60	14.257	1896	1899	1905	rVB4	17552	28368	0.52%	0.050%

61	14.375	1913	1919	1924	rBV	121355	174622	3.17%	0.310%
62	14.504	1934	1941	1949	rBV	1086107	1646172	29.89%	2.921%
63	14.593	1952	1956	1962	rVB9	7347	13569	0.25%	0.024%
64	14.716	1971	1977	1984	rBV2	133401	269590	4.89%	0.478%
65	15.098	2034	2042	2050	rVB6	12109	31546	0.57%	0.056%

66	15.193	2050	2058	2062	rBV3	20113	40304	0.73%	0.072%
67	15.322	2074	2080	2087	rBV4	33062	81059	1.47%	0.144%
68	15.498	2103	2110	2124	rBV	2839738	4089073	74.24%	7.256%
69	15.622	2125	2131	2141	rBV	900604	1275695	23.16%	2.264%
70	15.734	2147	2150	2156	rVB2	15941	24685	0.45%	0.044%

71	15.869	2167	2173	2185	rBV2	45374	73770	1.34%	0.131%
72	16.281	2240	2243	2248	rVB5	10039	13050	0.24%	0.023%
73	16.340	2248	2253	2258	rVB6	8305	13765	0.25%	0.024%
74	16.857	2337	2341	2345	rBV5	10033	13956	0.25%	0.025%
75	17.251	2399	2408	2418	rBV	1283858	1888085	34.28%	3.350%

76	17.357	2418	2426	2439	rBV	3292987	4768612	86.58%	8.462%
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77	17.557	2455	2460	2464	rBV	25233	34553	0.63%	0.061%
78	17.934	2519	2524	2531	rVV	550986	722870	13.12%	1.283%
79	18.104	2549	2553	2559	rBV5	13941	22376	0.41%	0.040%
80	18.163	2559	2563	2568	rVV2	33159	47668	0.87%	0.085%
81	18.245	2572	2577	2589	rVB2	39957	78356	1.42%	0.139%
82	18.375	2594	2599	2603	rVV	65482	89074	1.62%	0.158%
83	18.422	2603	2607	2610	rVV5	12082	19111	0.35%	0.034%
84	18.457	2610	2613	2616	rVV4	13546	20266	0.37%	0.036%
85	18.498	2617	2620	2628	rVB9	9423	16539	0.30%	0.029%
86	18.610	2634	2639	2643	rBV6	14559	23568	0.43%	0.042%
87	18.675	2647	2650	2655	rVV7	13627	27111	0.49%	0.048%
88	19.216	2738	2742	2747	rBV2	42970	59546	1.08%	0.106%
89	19.286	2748	2754	2759	rBV	35625	53782	0.98%	0.095%
90	19.451	2778	2782	2789	rBV7	21016	30646	0.56%	0.054%
91	19.610	2805	2809	2811	rBV4	17063	21133	0.38%	0.038%
92	19.657	2811	2817	2825	rVV	3858686	5507866	100.00%	9.774%
93	20.675	2985	2990	2996	rBV	298985	389780	7.08%	0.692%
94	21.457	3117	3123	3129	rBV	1448554	1895201	34.41%	3.363%
95	22.580	3310	3314	3323	rBV3	208372	362465	6.58%	0.643%
96	23.145	3406	3410	3415	rVB3	71142	108261	1.97%	0.192%
97	23.669	3491	3499	3511	rBV	2736907	5453448	99.01%	9.677%
98	23.769	3512	3516	3518	rVV2	105604	174777	3.17%	0.310%
99	23.816	3518	3524	3536	rVB	984413	2019894	36.67%	3.584%
100	24.486	3635	3638	3647	rVB3	83254	164511	2.99%	0.292%

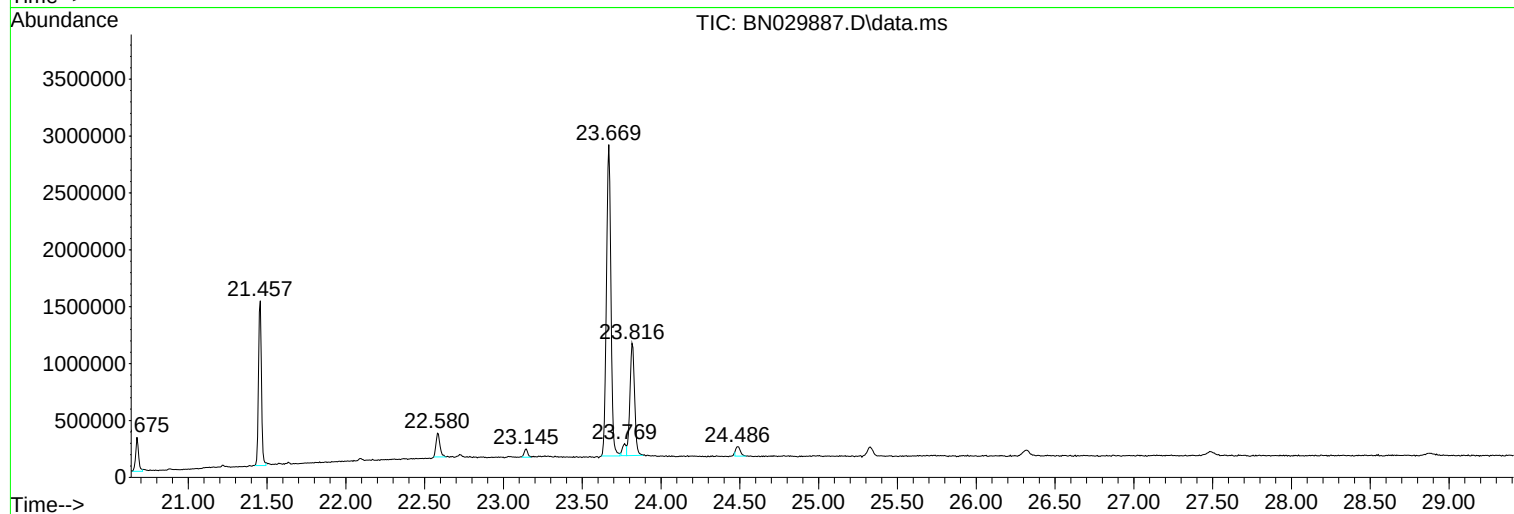
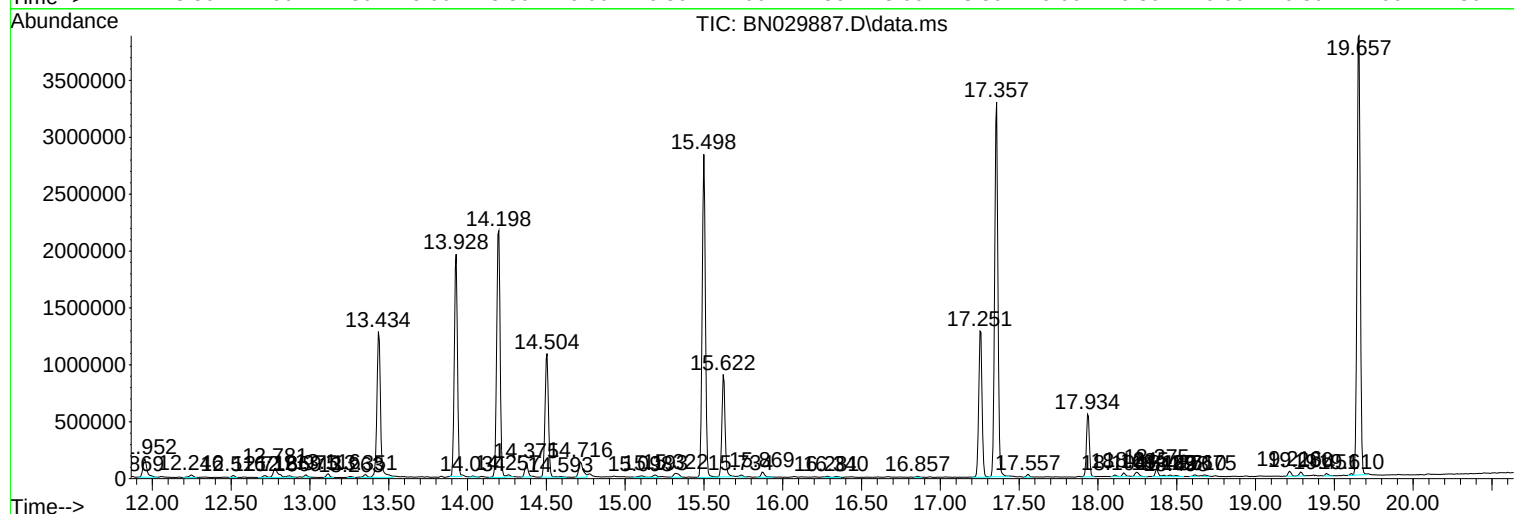
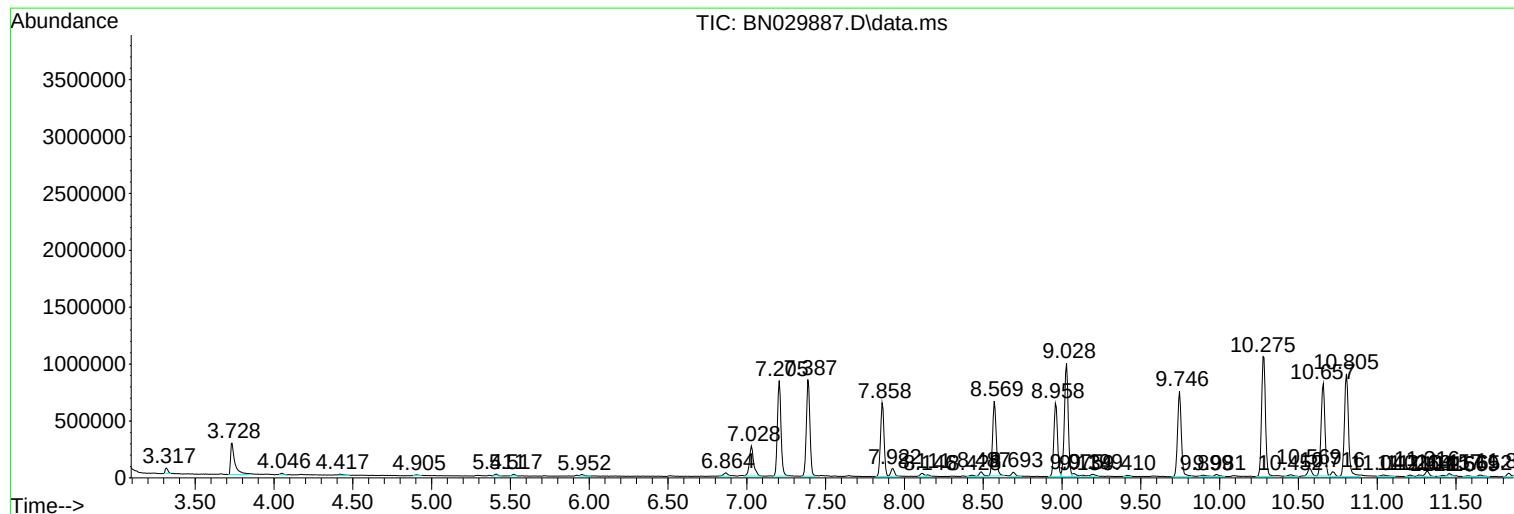
Sum of corrected areas: 56352427

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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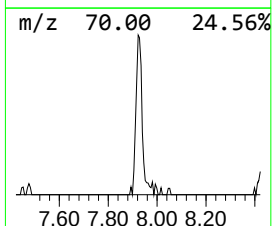
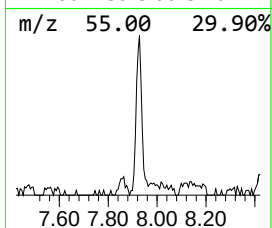
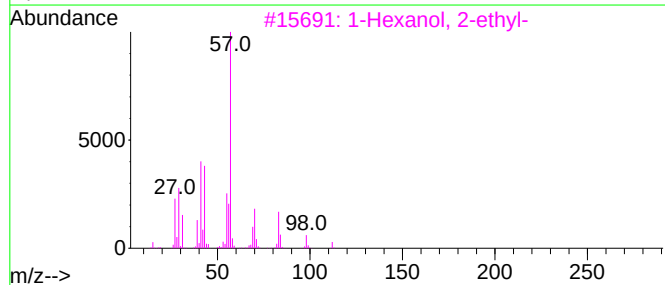
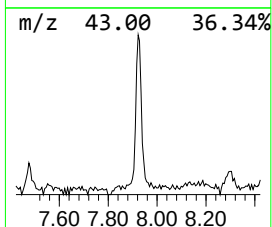
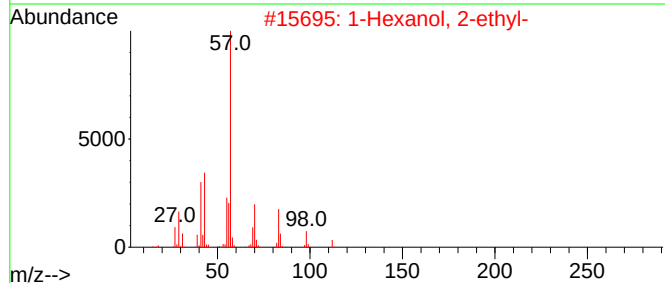
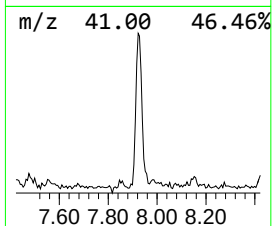
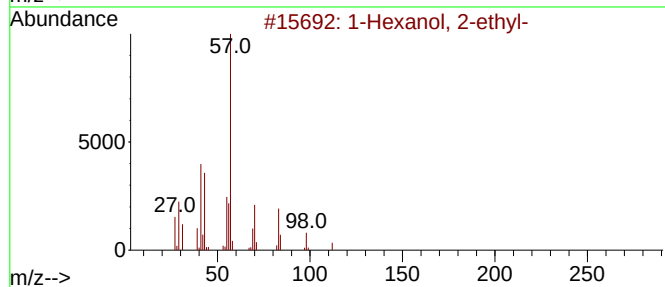
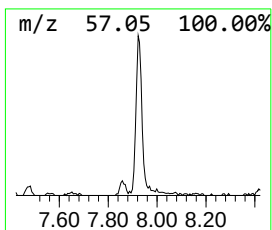
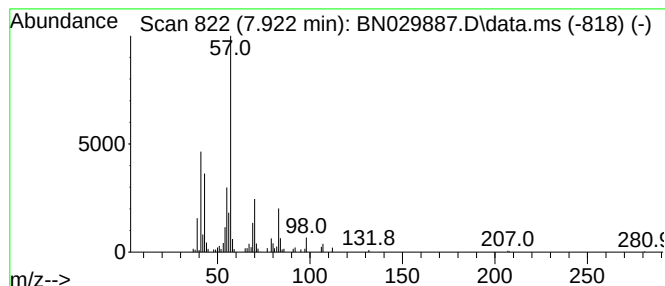
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.922	2.19 ng/ul	110986	1,4-Dichlorobenzene-d4	7.858

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59
4	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	50
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50



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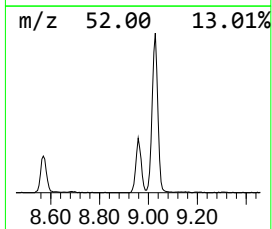
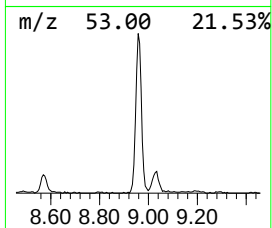
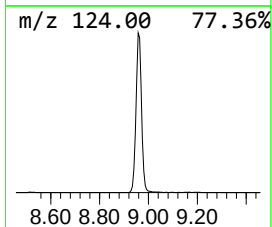
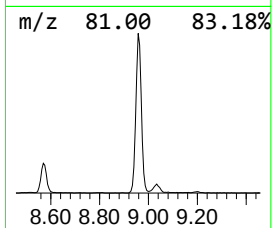
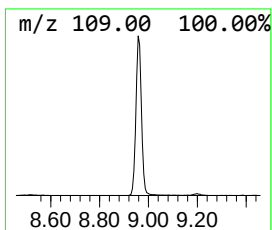
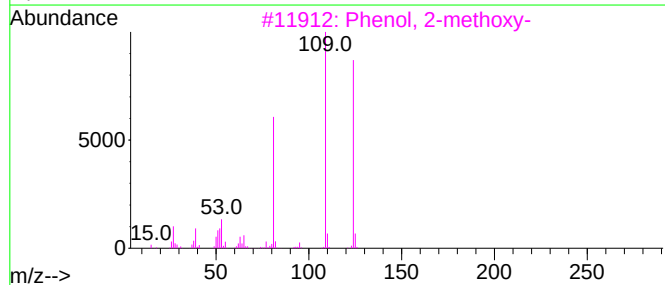
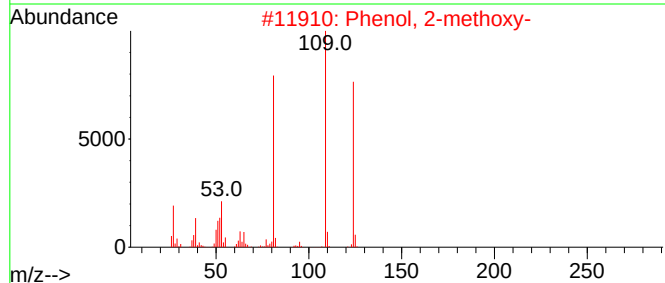
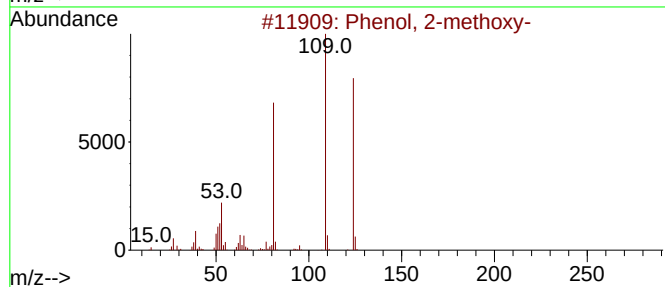
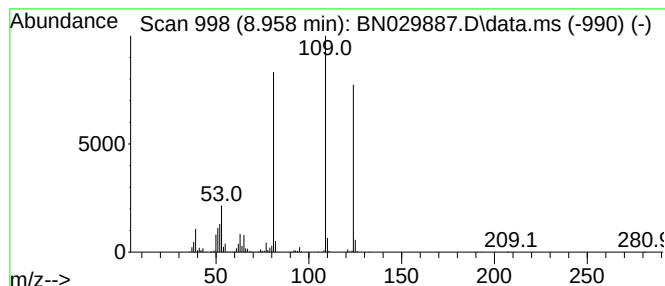
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	20.53 ng/ul	1039340	1,4-Dichlorobenzene-d4	7.858

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
4			Mequinol	124	C7H8O2	000150-76-5	91
5			Mequinol	124	C7H8O2	000150-76-5	90



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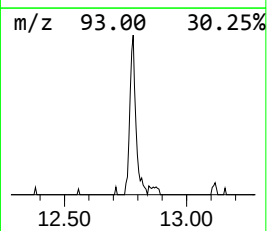
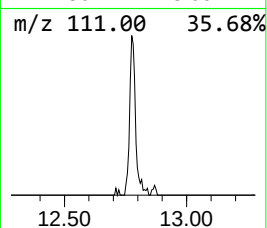
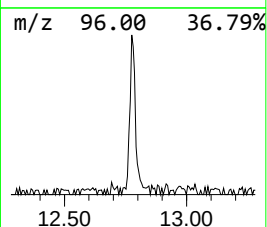
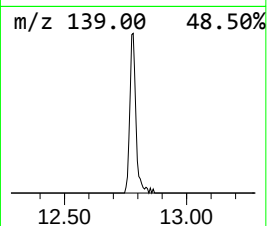
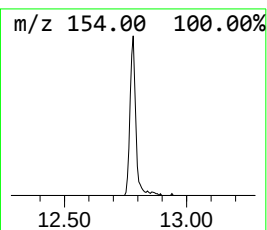
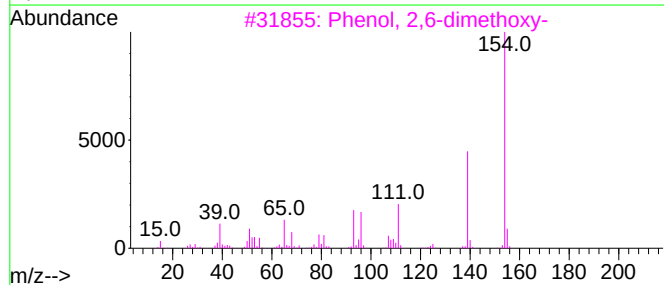
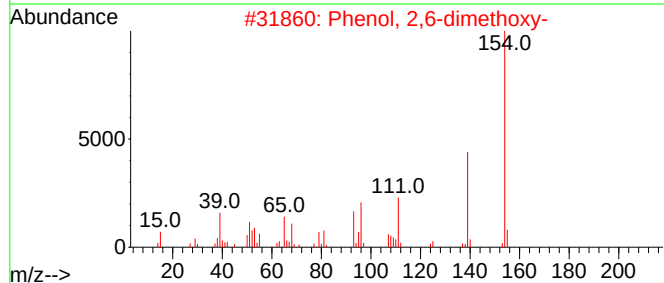
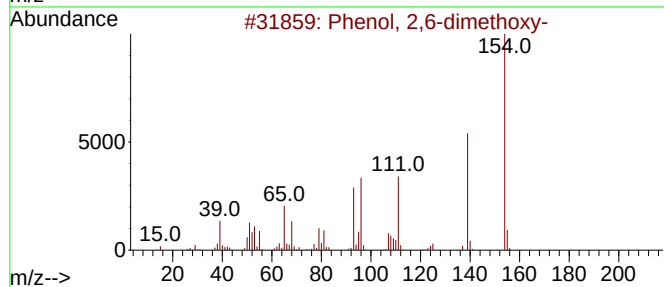
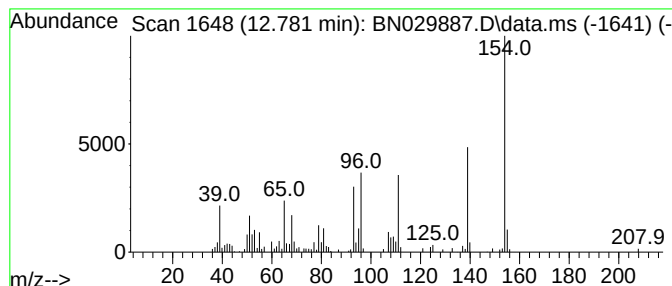
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenol, 2,6-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.781	2.14 ng/ul	176374	Acenaphthene-d10	14.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	98
2			Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	97
3			Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	96
4			Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	91
5			3-Amino-2,6-dimethoxypyridine	154	C7H10N2O2	028020-37-3	70



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Acq On : 21 Feb 2024 13:16
Operator : MA/JU
Sample : P1456-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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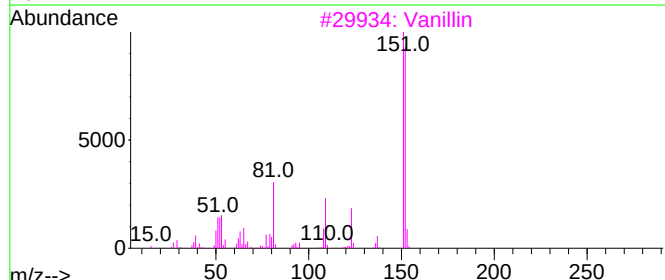
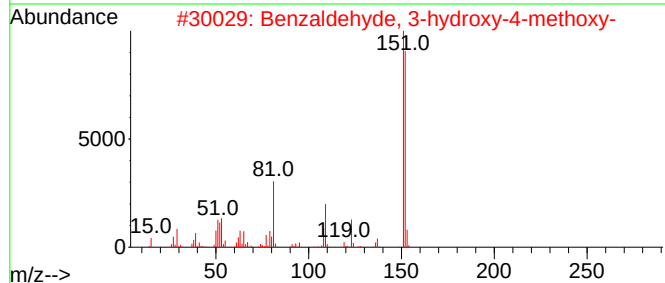
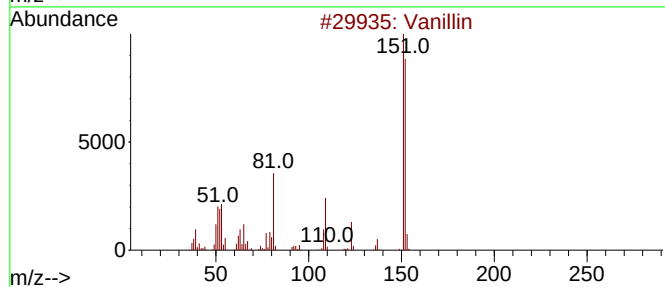
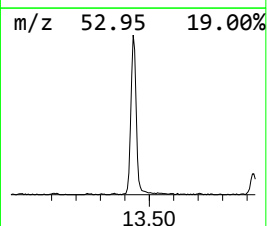
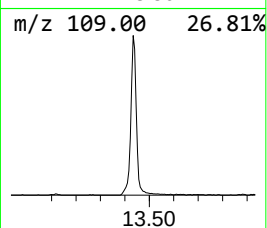
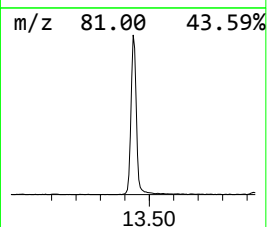
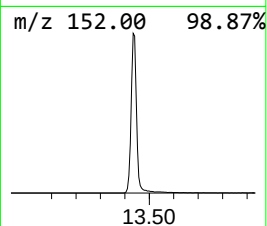
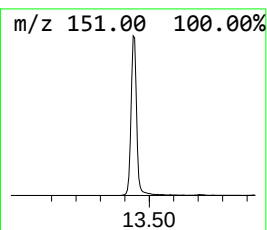
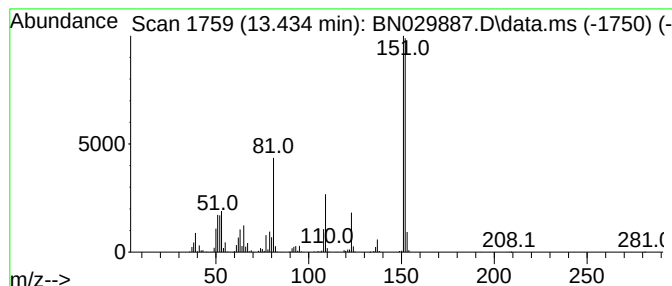
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.434	24.41 ng/ul	2009440	Acenaphthene-d10	14.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	97
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3			Vanillin	152	C8H8O3	000121-33-5	97
4			Vanillin	152	C8H8O3	000121-33-5	97
5			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
Data File : BN029887.D
Acq On : 21 Feb 2024 13:16
Operator : MA/JU
Sample : P1456-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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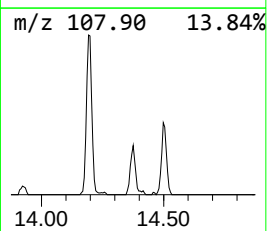
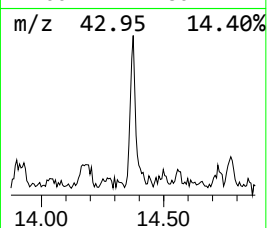
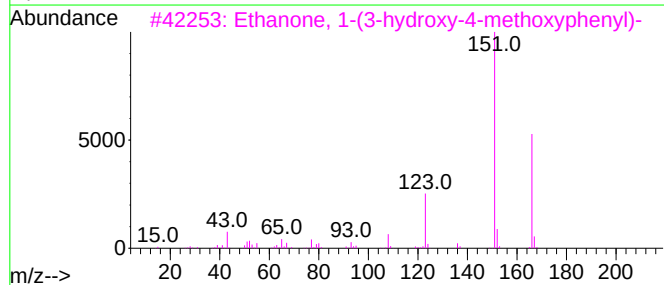
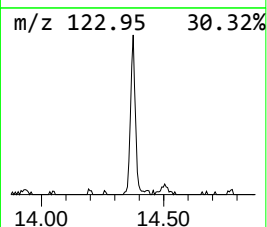
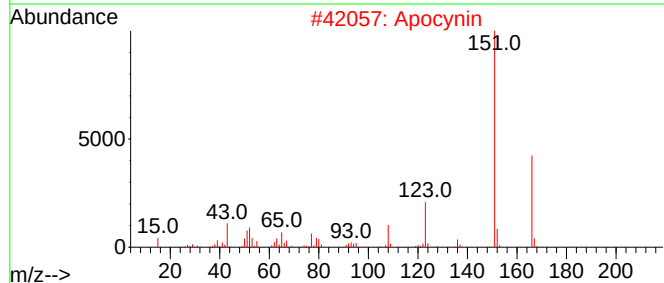
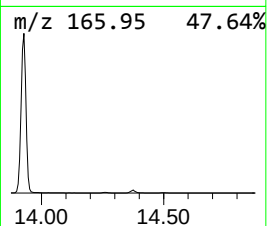
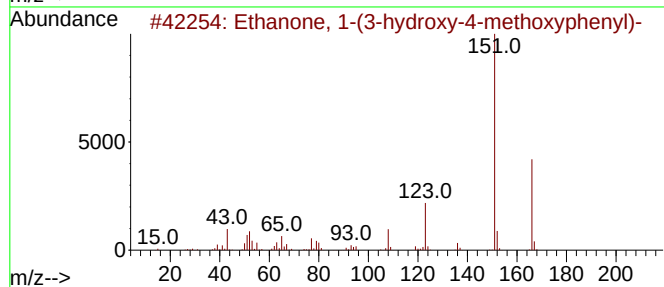
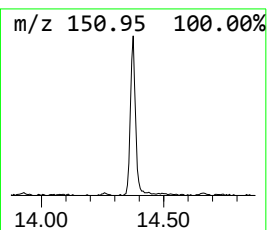
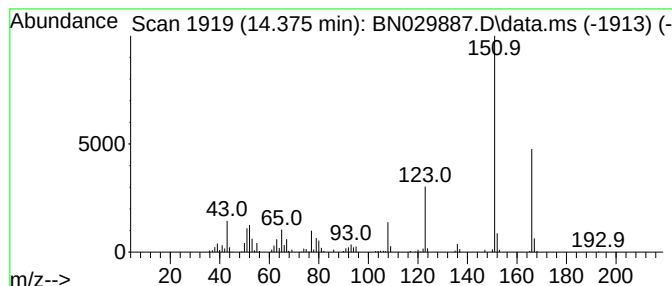
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanone, 1-(3-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.375	2.12 ng/ul	174622	Acenaphthene-d10	14.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	95
2			Apocynin	166	C9H10O3	000498-02-2	94
3			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	94
4			Apocynin	166	C9H10O3	000498-02-2	94
5			Apocynin	166	C9H10O3	000498-02-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
Data File : BN029887.D
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Operator : MA/JU
Sample : P1456-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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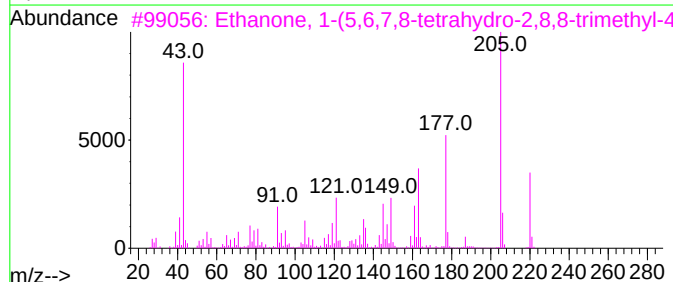
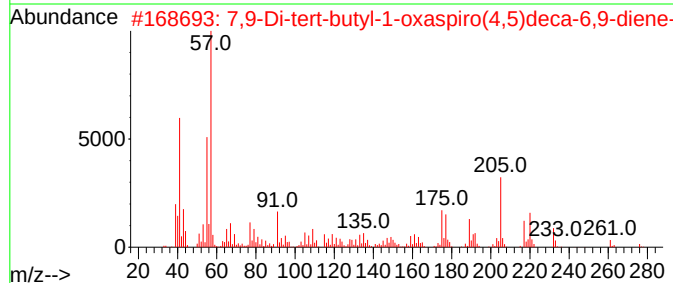
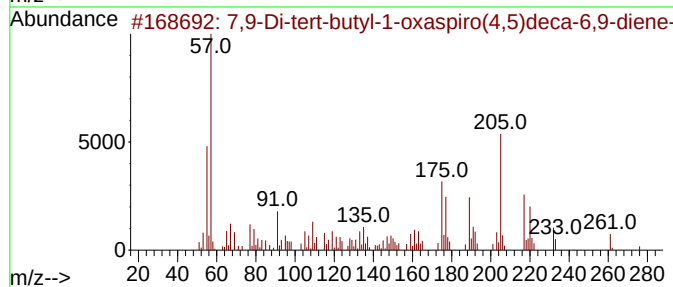
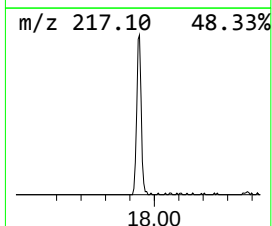
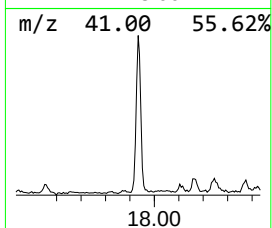
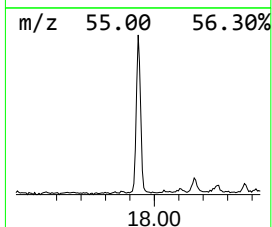
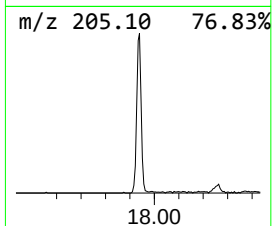
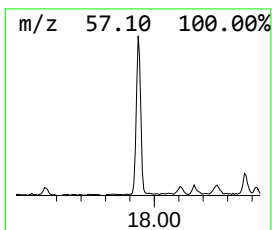
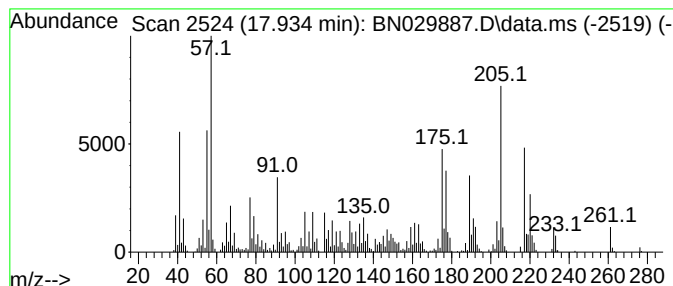
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	7.66 ng/ul	722870	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60		
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50		
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	50		
5	1,3,5-Cycloheptatriene, 2,4-di-t...	232	C17H28	1000160-92-5	46		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
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Sample : P1456-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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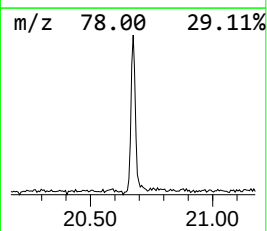
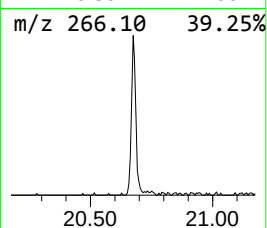
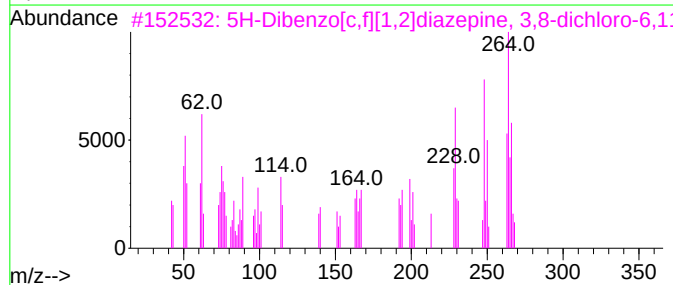
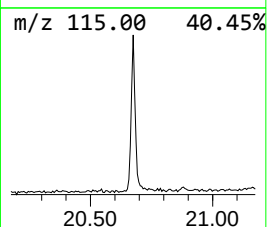
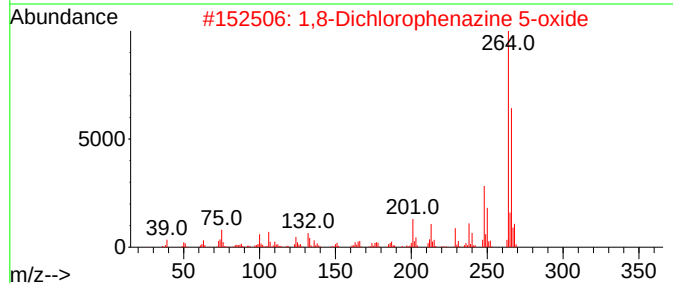
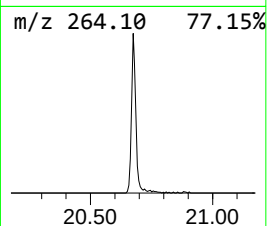
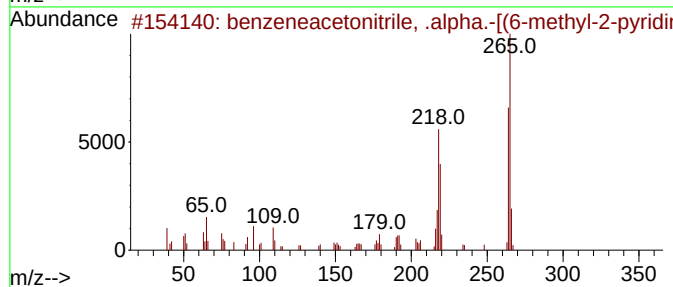
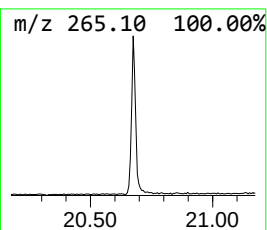
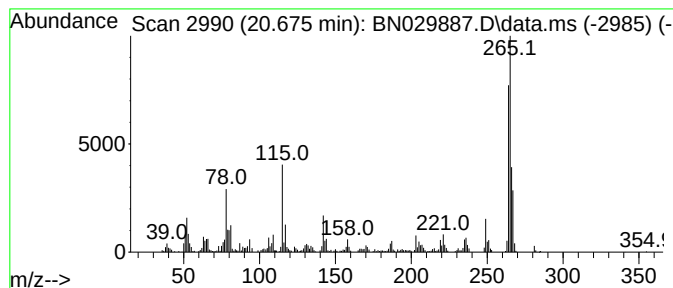
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.675	4.11 ng/ul	389780	Chrysene-d12	21.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			benzeneacetonitrile, .alpha.-[(6-methyl-2-pyridinyl)amino]benzo-	265	C15H11N3O2	1000396-89-7	38
2			1,8-Dichlorophenazine 5-oxide	264	C12H6Cl2N2O	006479-80-7	38
3			5H-Dibenzo[c,f][1,2]diazepine, 3,8-dichloro-6,11-dimethyl-	264	C13H10Cl2N2	000955-66-8	38
4			2,3-Bis(4-methoxyphenyl)prop-2-ene-1-thione	265	C17H15NO2	052565-72-7	38
5			5,6-Dimethyl-2-[(E)-2-(3-pyridinyl)vinyl]pyridine	266	C16H14N2S	897287-01-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
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Misc :
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Instrument :
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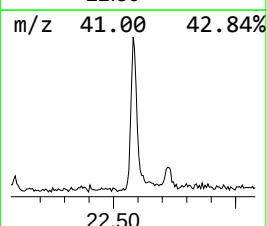
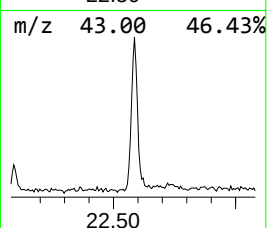
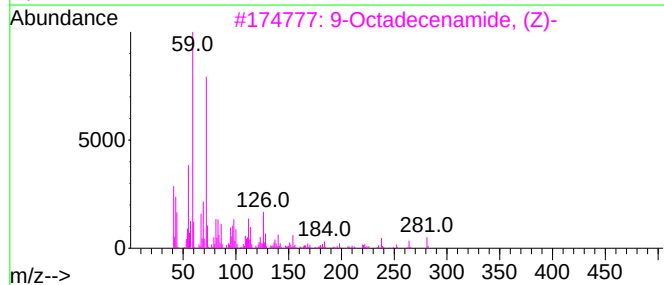
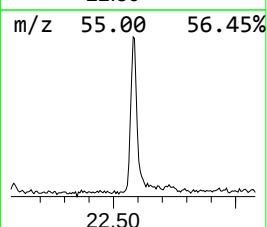
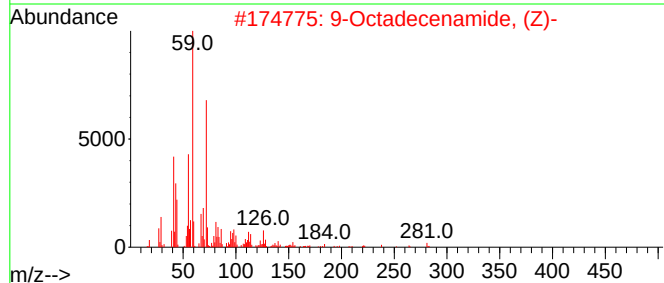
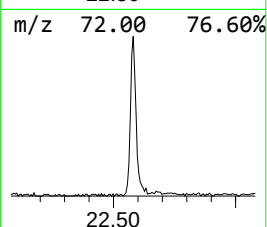
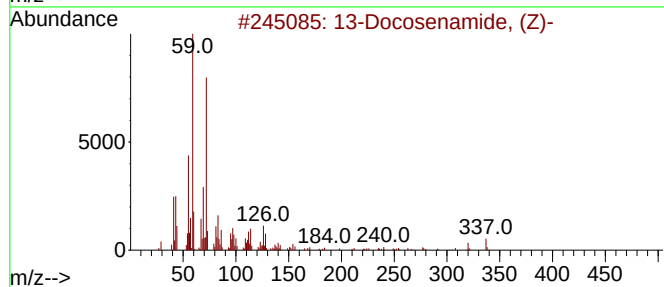
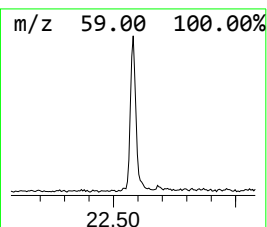
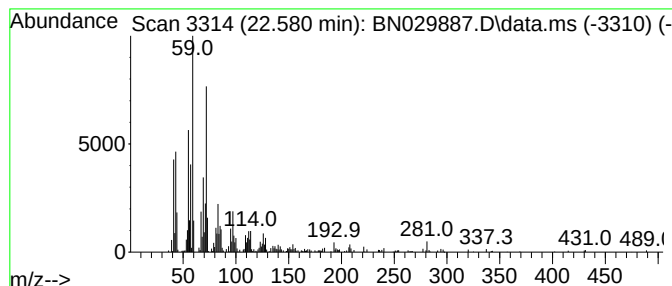
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.580	3.83 ng/ul	362465	Chrysene-d12	21.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
4			Palmitoleamide	253	C16H31NO	106010-22-4	64
5			9-Octadecenamide	281	C18H35NO	003322-62-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN022124\
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Operator : MA/JU
Sample : P1456-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	7.922	2.2	ng/ul	110986	1	7.858	1012340	20.0
Phenol, 2-methoxy-	8.958	20.5	ng/ul	1039340	1	7.858	1012340	20.0
Phenol, 2,6-dim...	12.781	2.1	ng/ul	176374	3	14.504	1646170	20.0
Vanillin	13.434	24.4	ng/ul	2009440	3	14.504	1646170	20.0
Ethanone, 1-(3-...	14.375	2.1	ng/ul	174622	3	14.504	1646170	20.0
7,9-Di-tert-but...	17.933	7.7	ng/ul	722870	4	17.257	1888090	20.0
unknown-01	20.675	4.1	ng/ul	389780	5	21.457	1895200	20.0
13-Docosenamide...	22.580	3.8	ng/ul	362465	5	21.457	1895200	20.0