

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
 Data File : BP022214.D
 Acq On : 04 Oct 2024 04:42
 Operator : RC/JU
 Sample : P4017-11DL 30X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DDC86DL

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_P\Methods\SFAM-EPA-BP092424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP022214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.875	654	661	667	rBV6	8110	24587	0.25%	0.106%
2	7.034	683	688	693	rBV	7293	12996	0.13%	0.056%
3	7.134	701	705	711	rBV3	6581	10702	0.11%	0.046%
4	7.240	717	723	732	rVB3	9962	21902	0.23%	0.094%
5	7.346	732	741	749	rVB2	13280	28340	0.29%	0.122%
6	7.616	778	787	791	rBV9	4676	12917	0.13%	0.055%
7	7.693	791	800	809	rBV	364840	613037	6.30%	2.632%
8	8.328	902	908	915	rBV5	7550	21330	0.22%	0.092%
9	8.399	915	920	924	rVV6	7575	15158	0.16%	0.065%
10	8.446	924	928	932	rVV2	10015	14987	0.15%	0.064%
11	8.634	955	960	963	rBV2	6827	10578	0.11%	0.045%
12	8.675	963	967	975	rVB5	13920	26612	0.27%	0.114%
13	8.787	981	986	991	rVV5	10293	18263	0.19%	0.078%
14	8.840	991	995	999	rVV2	6539	11093	0.11%	0.048%
15	8.905	1002	1006	1011	rVB	15562	24590	0.25%	0.106%
16	9.022	1016	1026	1032	rVB9	9786	23189	0.24%	0.100%
17	9.257	1056	1066	1069	rBV9	4131	10475	0.11%	0.045%
18	9.363	1079	1084	1087	rBV3	7684	11771	0.12%	0.051%
19	9.452	1092	1099	1106	rVB4	11600	21157	0.22%	0.091%
20	9.552	1109	1116	1120	rBV7	8642	16824	0.17%	0.072%
21	9.675	1129	1137	1141	rBV8	5928	12714	0.13%	0.055%
22	9.810	1154	1160	1164	rBV8	5736	10717	0.11%	0.046%
23	9.869	1164	1170	1175	rVV8	9508	24794	0.25%	0.106%
24	9.934	1177	1181	1186	rVB2	6333	10748	0.11%	0.046%
25	10.093	1204	1208	1214	rBV4	8107	14382	0.15%	0.062%
26	10.452	1257	1269	1278	rBV2	722739	1326091	13.63%	5.693%
27	10.569	1283	1289	1303	rVB	123236	213344	2.19%	0.916%
28	10.728	1310	1316	1324	rBV6	18020	38855	0.40%	0.167%
29	10.846	1329	1336	1341	rBV7	10936	18960	0.19%	0.081%
30	10.957	1347	1355	1362	rBV	89599	138208	1.42%	0.593%
31	11.340	1415	1420	1424	rBV2	22066	36966	0.38%	0.159%
32	11.487	1438	1445	1450	rBV6	8560	17262	0.18%	0.074%
33	11.569	1454	1459	1464	rBV4	10347	17272	0.18%	0.074%
34	11.681	1473	1478	1482	rBV6	16811	32239	0.33%	0.138%
35	11.793	1491	1497	1503	rBV4	13406	23835	0.25%	0.102%
36	11.875	1505	1511	1517	rVV	39093	58432	0.60%	0.251%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
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37	12.004	1527	1533	1538	rVB8	9334	18986	0.20%	0.082%
38	12.116	1546	1552	1560	rVB	22459	36944	0.38%	0.159%
39	12.228	1563	1571	1575	rBV4	14689	27242	0.28%	0.117%
40	12.287	1575	1581	1586	rVV3	110734	220589	2.27%	0.947%

41	12.334	1586	1589	1598	rVB2	33259	50738	0.52%	0.218%
42	12.493	1609	1616	1619	rBV6	5889	12948	0.13%	0.056%
43	12.546	1621	1625	1632	rVB	19609	30553	0.31%	0.131%
44	12.634	1634	1640	1645	rBV5	24335	39957	0.41%	0.172%
45	12.687	1645	1649	1655	rVB3	9553	15952	0.16%	0.068%

46	12.757	1655	1661	1663	rBV5	6560	13111	0.13%	0.056%
47	12.828	1668	1673	1676	rVV4	7192	11806	0.12%	0.051%
48	12.875	1676	1681	1686	rVB3	41031	66875	0.69%	0.287%
49	12.928	1686	1690	1696	rBV3	12578	19797	0.20%	0.085%
50	13.022	1701	1706	1712	rBV9	9712	19653	0.20%	0.084%

51	13.122	1719	1723	1729	rVB3	33159	53664	0.55%	0.230%
52	13.187	1729	1734	1736	rBV5	12601	18132	0.19%	0.078%
53	13.257	1742	1746	1754	rVB2	16075	30825	0.32%	0.132%
54	13.346	1754	1761	1772	rVB4	72675	150485	1.55%	0.646%
55	13.481	1772	1784	1789	rBV4	50068	135408	1.39%	0.581%

56	13.522	1789	1791	1798	rVB5	12641	17268	0.18%	0.074%
57	13.616	1798	1807	1811	rBV3	49959	104460	1.07%	0.448%
58	13.710	1819	1823	1828	rVB	24015	41528	0.43%	0.178%
59	13.857	1840	1848	1851	rBV5	17247	32306	0.33%	0.139%
60	13.993	1867	1871	1873	rBV	22013	28323	0.29%	0.122%

61	14.028	1873	1877	1883	rVB	32419	50329	0.52%	0.216%
62	14.104	1887	1890	1895	rVB6	14846	20832	0.21%	0.089%
63	14.210	1903	1908	1912	rBV	63333	85041	0.87%	0.365%
64	14.263	1912	1917	1918	rBV3	20599	26381	0.27%	0.113%
65	14.304	1918	1924	1931	rVB	787623	1211741	12.46%	5.202%

66	14.522	1958	1961	1964	rBV5	7038	10175	0.10%	0.044%
67	14.563	1964	1968	1972	rVB2	23264	30423	0.31%	0.131%
68	14.604	1972	1975	1981	rBV6	10950	20527	0.21%	0.088%
69	14.704	1989	1992	2001	rVB3	22379	33861	0.35%	0.145%
70	14.787	2001	2006	2010	rBV3	12533	23483	0.24%	0.101%

71	14.863	2010	2019	2023	rBV8	22846	49013	0.50%	0.210%
72	14.945	2027	2033	2042	rVB	942680	1273602	13.09%	5.468%
73	15.034	2043	2048	2049	rBV2	9235	14577	0.15%	0.063%
74	15.151	2063	2068	2069	rBV3	7888	10878	0.11%	0.047%
75	15.181	2069	2073	2078	rVB	30969	39722	0.41%	0.171%

76	15.310	2091	2095	2099	rVB	45791	56244	0.58%	0.241%
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 Title : SVOA CALIBRATION

77	15.398	2106	2110	2111	rBV3	14713	16734	0.17%	0.072%
78	15.592	2139	2143	2151	rVB4	24792	47411	0.49%	0.204%
79	15.687	2154	2159	2165	rVB4	32282	50592	0.52%	0.217%
80	15.898	2191	2195	2198	rBV5	7362	11951	0.12%	0.051%
81	16.045	2216	2220	2233	rVB2	34022	73112	0.75%	0.314%
82	16.157	2234	2239	2244	rBV6	15030	29786	0.31%	0.128%
83	16.275	2253	2259	2263	rBV9	6142	10781	0.11%	0.046%
84	16.745	2332	2339	2353	rBV	7204943	9727176	100.00%	41.761%
85	16.869	2357	2360	2365	rVV	49939	83323	0.86%	0.358%
86	16.928	2367	2370	2379	rVB2	30152	50261	0.52%	0.216%
87	17.098	2393	2399	2405	rBV	1107530	1588243	16.33%	6.819%
88	17.139	2405	2406	2411	rVB	39631	37669	0.39%	0.162%
89	17.204	2411	2417	2423	rVB2	39802	67776	0.70%	0.291%
90	17.634	2486	2490	2494	rBV	33125	42850	0.44%	0.184%
91	17.704	2498	2502	2505	rVB2	14485	19900	0.20%	0.085%
92	18.010	2550	2554	2556	rBV3	15045	21549	0.22%	0.093%
93	18.198	2582	2586	2590	rBV3	12374	18943	0.19%	0.081%
94	18.351	2608	2612	2620	rBV2	30762	47018	0.48%	0.202%
95	18.516	2637	2640	2644	rBV6	7770	13450	0.14%	0.058%
96	19.010	2721	2724	2730	rBV5	27213	38947	0.40%	0.167%
97	19.228	2758	2761	2766	rVB	18632	26059	0.27%	0.112%
98	19.575	2816	2820	2824	rBV	62177	98108	1.01%	0.421%
99	21.533	3147	3153	3159	rBV	1272566	1967648	20.23%	8.447%
100	24.810	3701	3710	3721	rVB	703632	2103721	21.63%	9.032%

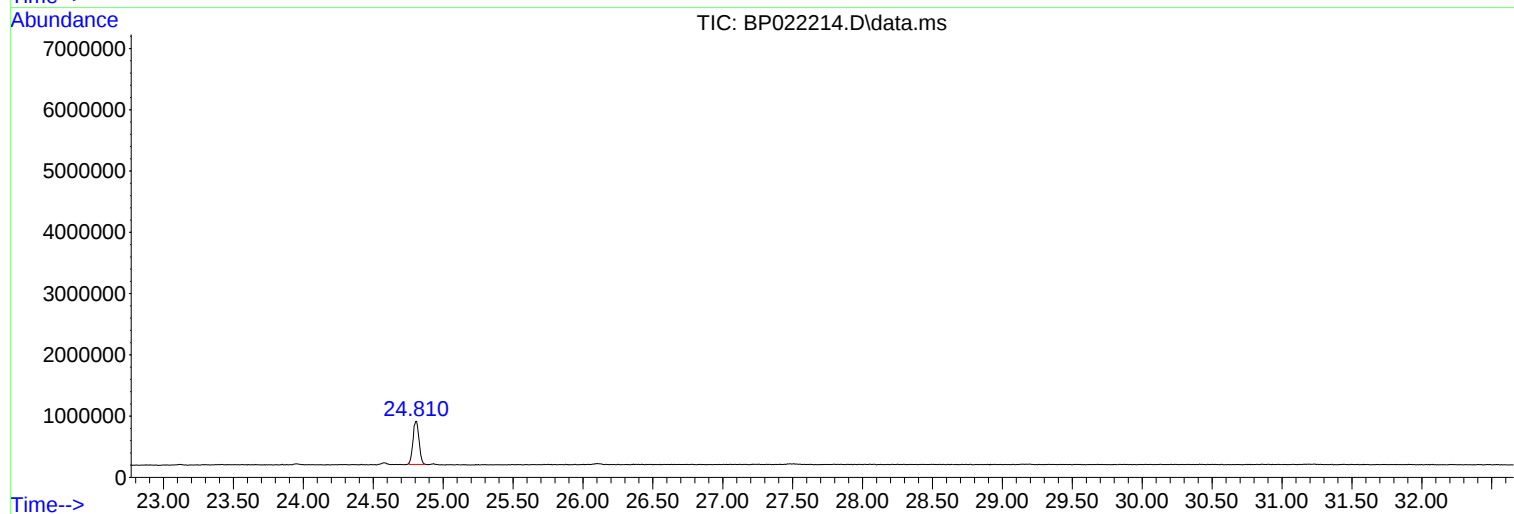
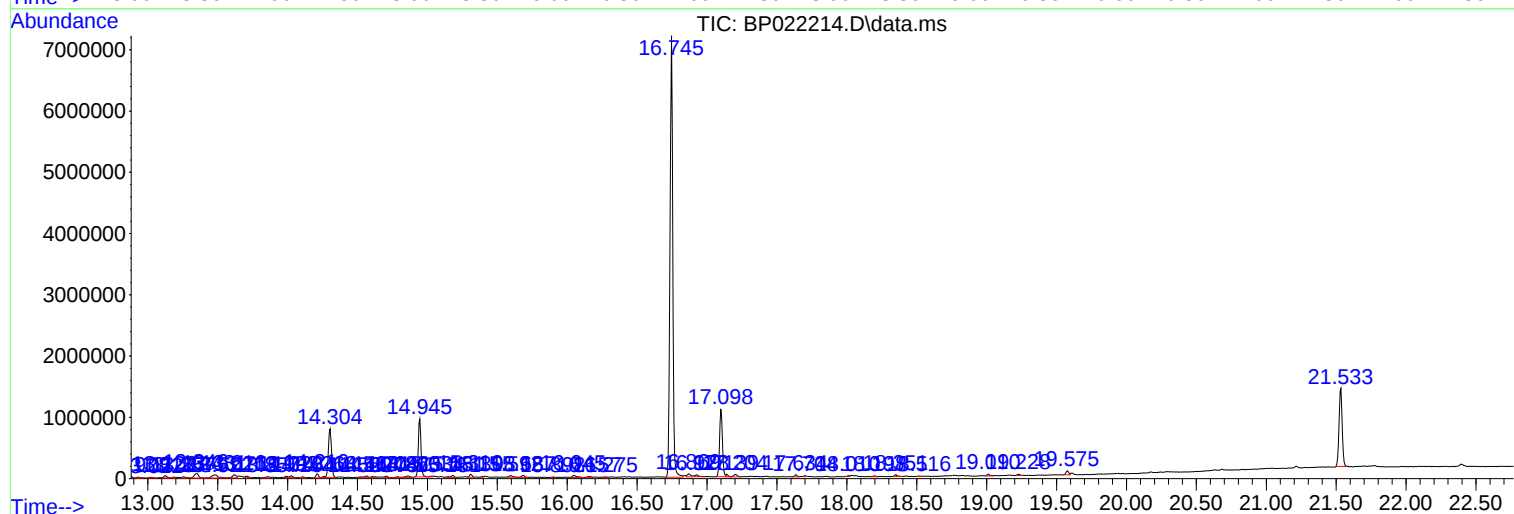
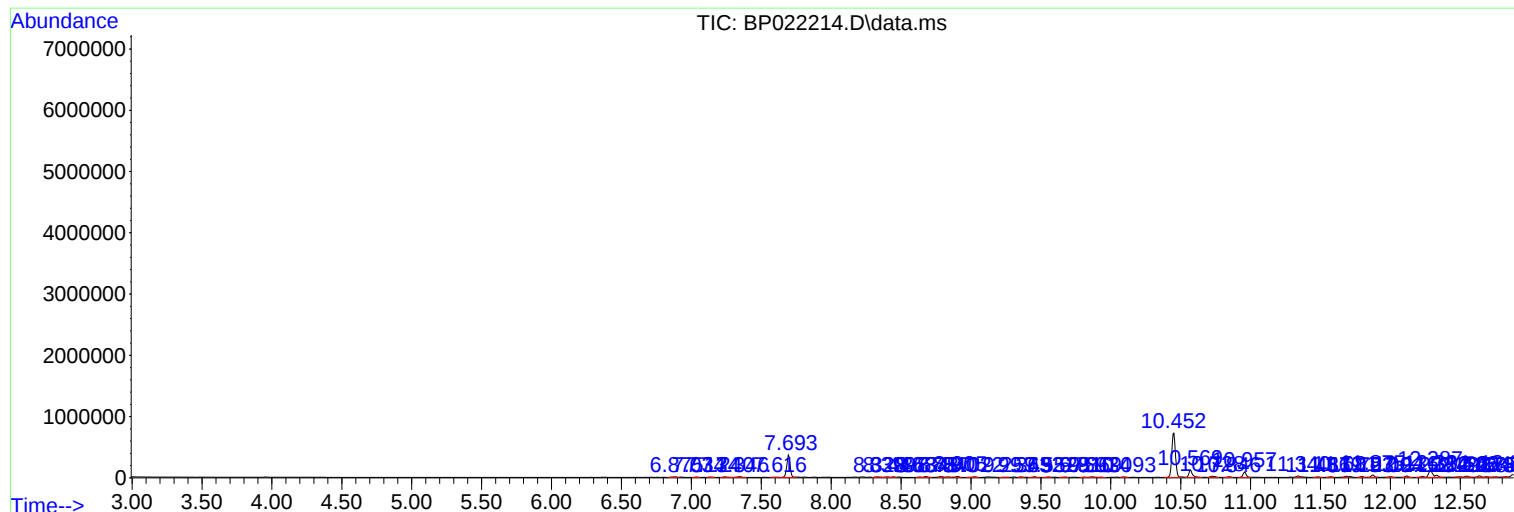
Sum of corrected areas: 23292714

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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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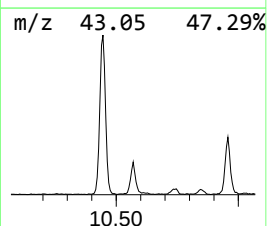
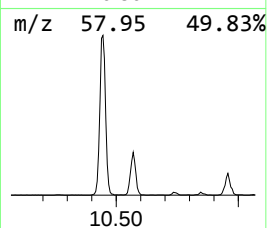
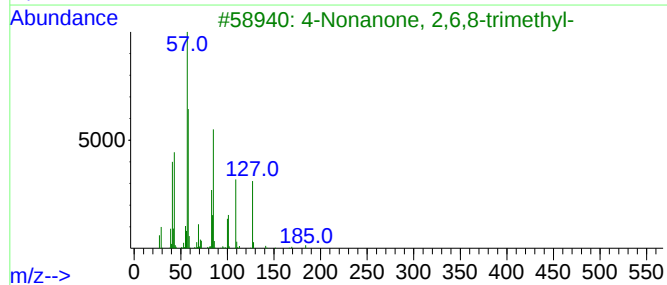
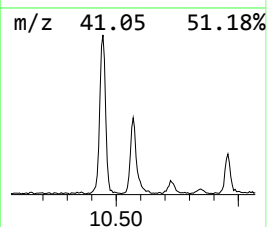
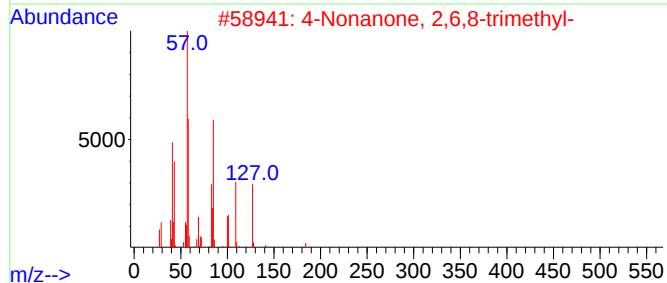
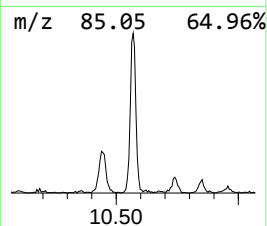
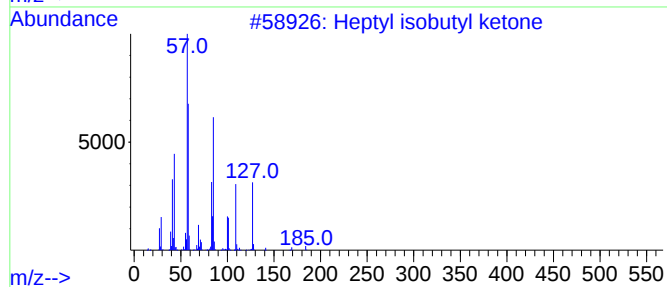
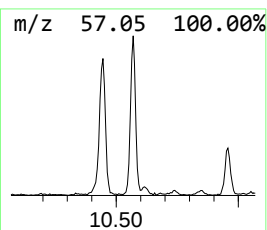
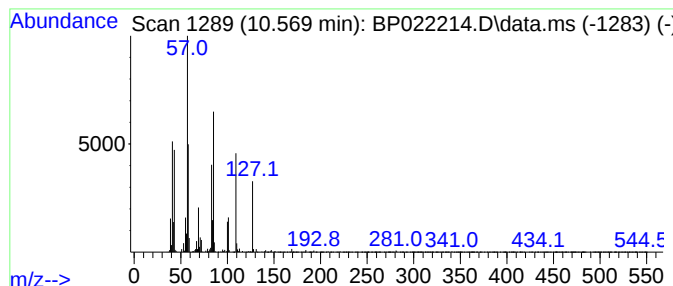
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Heptyl isobutyl ketone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	3.22 ng/ul	213344	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl ketone	184	C12H24O	019594-40-2	93
2			4-Nonanone, 2,6,8-trimethyl-	184	C12H24O	000123-18-2	72
3			4-Nonanone, 2,6,8-trimethyl-	184	C12H24O	000123-18-2	64
4			5-Dodecanone	184	C12H24O	019780-10-0	47
5			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	35



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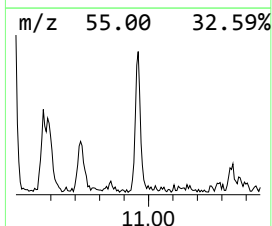
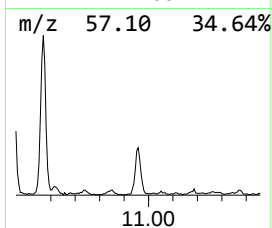
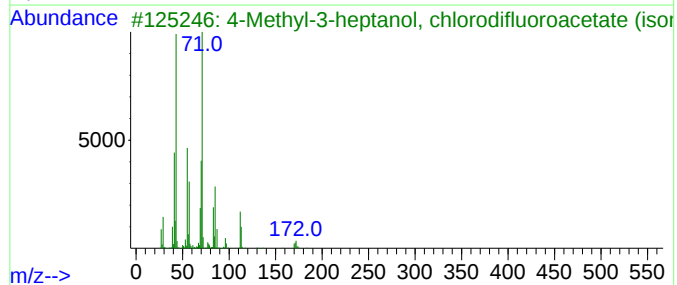
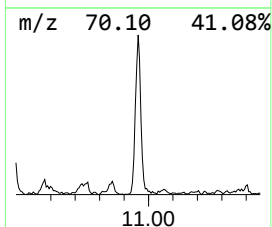
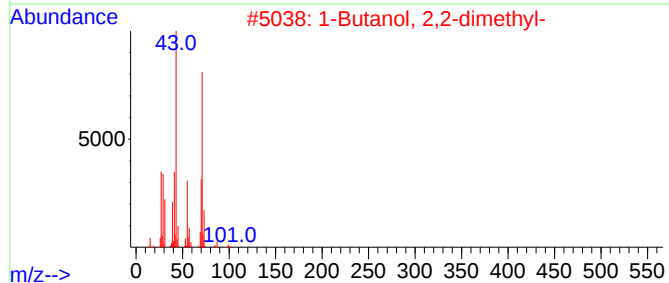
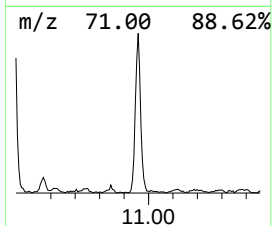
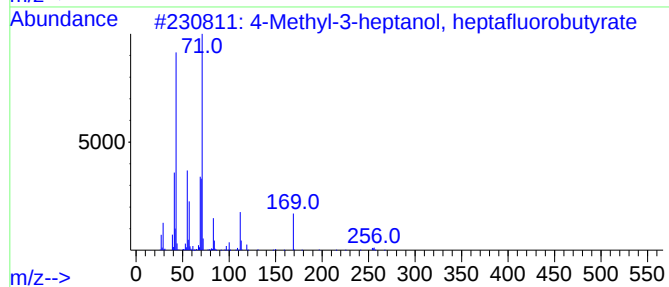
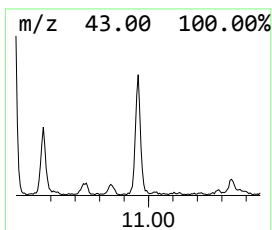
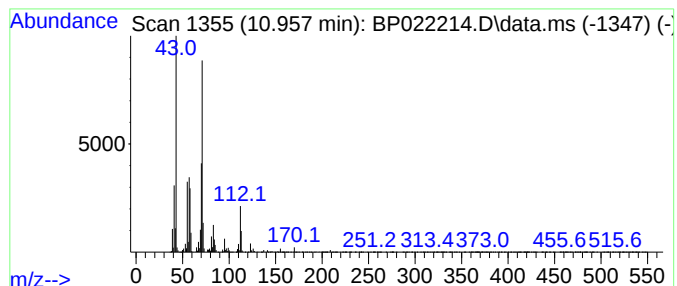
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 4-Methyl-3-heptanol, heptaf... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.957	2.08 ng/ul	138208	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-3-heptanol, heptafluoro...	326	C12H17F7O2	1000365-51-5	59
2			1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	47
3			4-Methyl-3-heptanol, chlorodiflu...	242	C10H17ClF2O2	1000447-28-3	45
4			3-Octen-2-ol	128	C8H16O	076649-14-4	43
5			Butyric acid, p-fluorophenyl ester	182	C10H11FO2	000587-89-3	43



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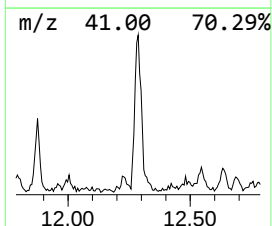
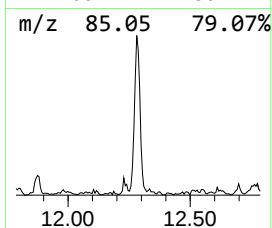
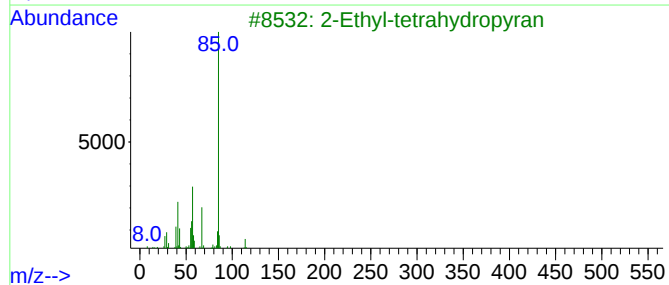
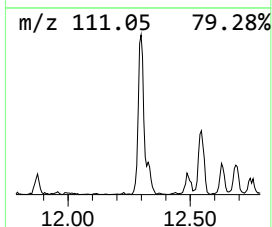
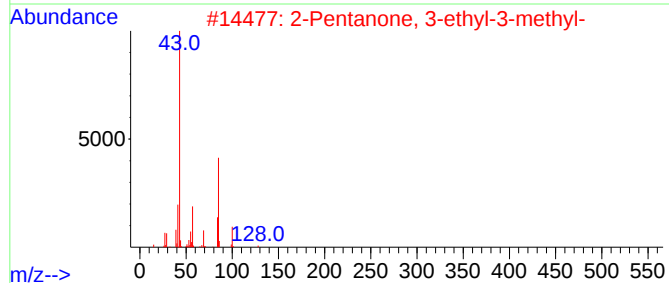
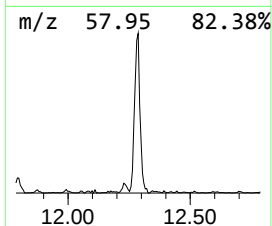
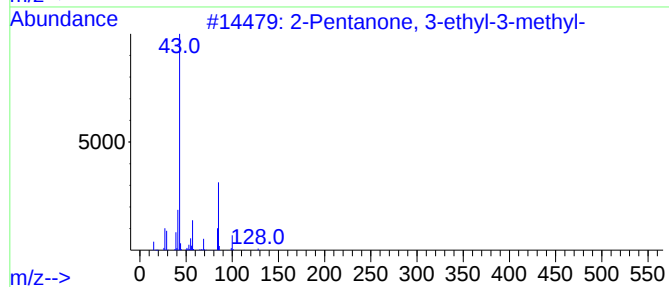
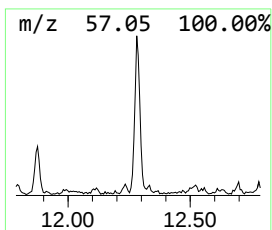
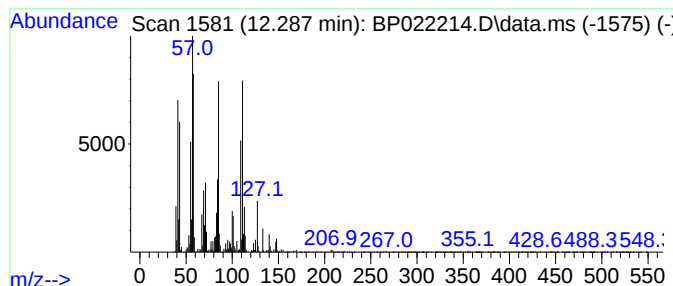
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.287	3.33 ng/ul	220589	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	14		
2	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	14		
3	2-Ethyl-tetrahydropyran	114	C7H14O	1000386-40-1	11		
4	Butanoic acid, 3-hydroxy-3-(2,2-...	301	C16H31NO4	1000265-23-0	11		
5	Cytosine	111	C4H5N3O	000071-30-7	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022214.D
Acq On : 04 Oct 2024 04:42
Operator : RC/JU
Sample : P4017-11DL 30X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DDC86DL

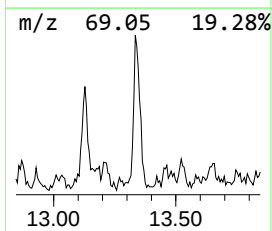
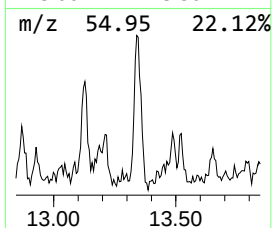
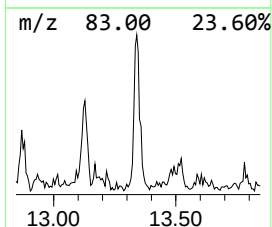
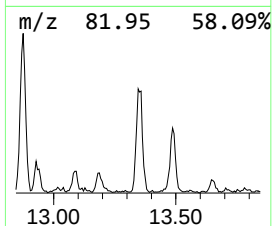
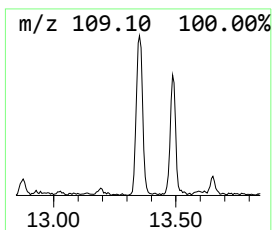
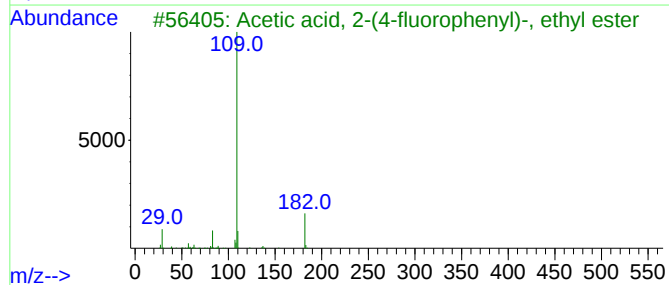
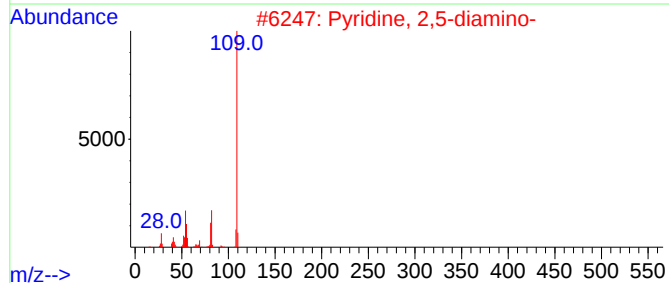
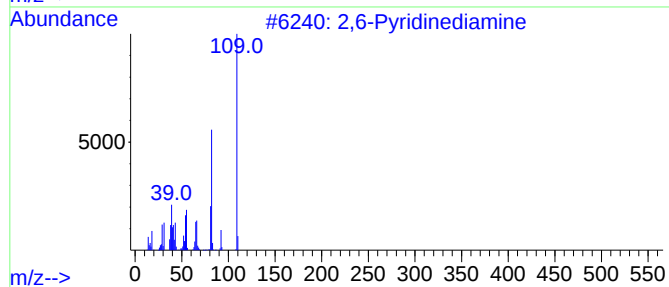
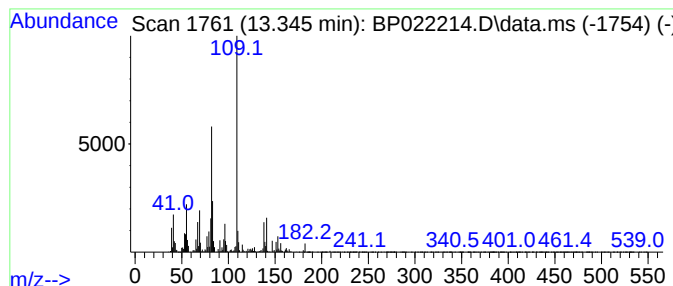
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 2,6-Pyridinediamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.345	2.48 ng/ul	150485	Acenaphthene-d10	14.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Pyridinediamine	109	C5H7N3	000141-86-6	50
2			Pyridine, 2,5-diamino-	109	C5H7N3	004318-76-7	43
3			Acetic acid, 2-(4-fluorophenyl)-...	182	C10H11F02	1000439-01-7	43
4			1,2,5-Oxadiazole-3-carboxamide, ...	279	C12H14FN5O2	1010319-53-8	38
5			Pyridine-2,4-diamine	109	C5H7N3	000461-88-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022214.D
Acq On : 04 Oct 2024 04:42
Operator : RC/JU
Sample : P4017-11DL 30X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DDC86DL

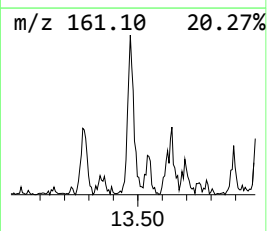
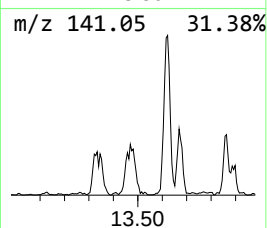
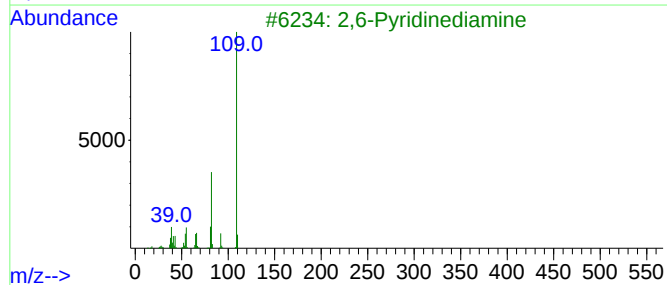
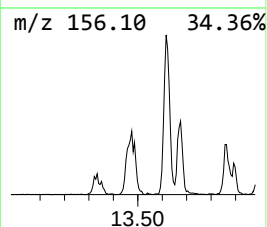
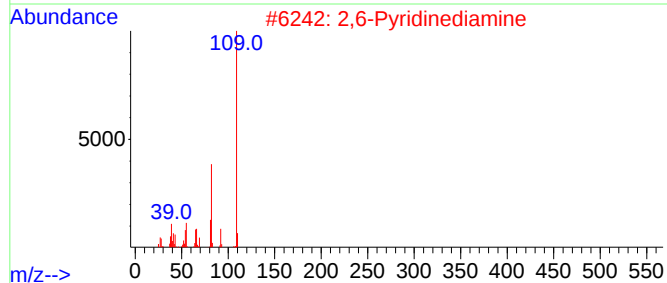
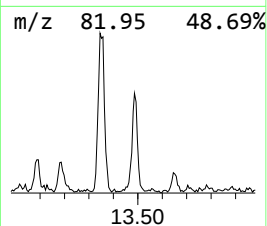
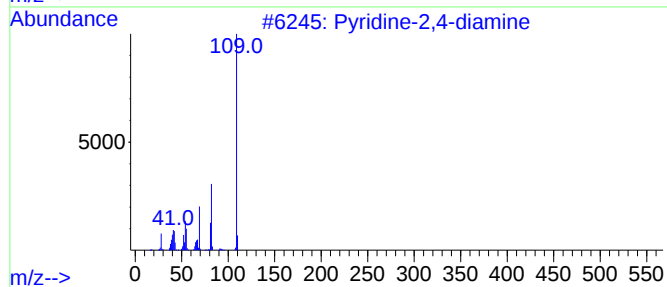
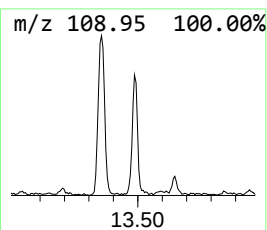
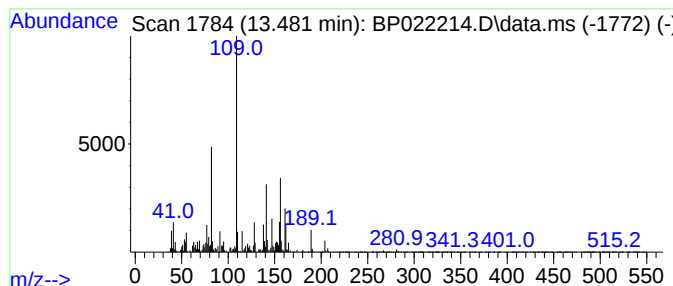
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.481	2.23 ng/ul	135408	Acenaphthene-d10	14.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine-2,4-diamine	109	C5H7N3	000461-88-1	38
2			2,6-Pyridinediamine	109	C5H7N3	000141-86-6	38
3			2,6-Pyridinediamine	109	C5H7N3	000141-86-6	38
4			Pyridine, 2,5-diamino-	109	C5H7N3	004318-76-7	30
5			2,3-Pyridinediamine	109	C5H7N3	000452-58-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022214.D
Acq On : 04 Oct 2024 04:42
Operator : RC/JU
Sample : P4017-11DL 30X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DDC86DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
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
Heptyl isobutyl...	10.569	3.2	ng/u1	213344	2	10.451	1326090	20.0
4-Methyl-3-hept...	10.957	2.1	ng/u1	138208	2	10.451	1326090	20.0
unknown-01	12.287	3.3	ng/u1	220589	2	10.451	1326090	20.0
2,6-Pyridinedia...	13.345	2.5	ng/u1	150485	3	14.304	1211740	20.0
unknown-02	13.481	2.2	ng/u1	135408	3	14.304	1211740	20.0