

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060721\
 Data File : BF124168.D
 Acq On : 7 Jun 2021 21:28
 Operator : JU/CG
 Sample : M2589-18 10X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(0-2)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_F\METHODS\8270-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.434	395	399	404	rBB	110469	118867	37.90%	5.153%
2	5.057	501	505	511	rVB	96603	90817	28.96%	3.937%
3	6.504	748	751	754	rBV	15922	12981	4.14%	0.563%
4	6.857	808	811	815	rBV	306460	244192	77.86%	10.585%
5	7.416	903	906	911	rBV	42237	34024	10.85%	1.475%
6	8.145	1026	1030	1033	rBV	353737	288994	92.15%	12.527%
7	9.216	1209	1212	1218	rBB	77879	55082	17.56%	2.388%
8	9.898	1325	1328	1332	rBV	422430	313610	100.00%	13.594%
9	10.816	1478	1484	1489	rVB2	3137	5517	1.76%	0.239%
10	11.245	1555	1557	1560	rBV	3856	4189	1.34%	0.182%
11	11.386	1577	1581	1584	rBV	345255	285209	90.94%	12.363%
12	11.674	1625	1630	1632	rVB2	3630	4437	1.41%	0.192%
13	11.721	1635	1638	1641	rVB	3579	4220	1.35%	0.183%
14	11.769	1641	1646	1648	rBV2	4322	6671	2.13%	0.289%
15	11.921	1665	1672	1674	rBV4	5187	11669	3.72%	0.506%
16	12.080	1696	1699	1702	rBV2	4005	5011	1.60%	0.217%
17	12.210	1718	1721	1723	rVB3	5458	4250	1.36%	0.184%
18	12.433	1756	1759	1760	rBV3	3601	4487	1.43%	0.195%
19	12.604	1785	1788	1791	rVB2	15340	14833	4.73%	0.643%
20	12.763	1813	1815	1816	rBV2	5518	4383	1.40%	0.190%
21	12.827	1824	1826	1832	rVB	14847	21066	6.72%	0.913%
22	12.916	1838	1841	1843	rBV4	4921	5190	1.65%	0.225%
23	12.968	1847	1850	1853	rBV	82989	69798	22.26%	3.026%
24	13.027	1858	1860	1861	rBV2	6242	4642	1.48%	0.201%
25	13.151	1879	1881	1883	rBV3	6558	4998	1.59%	0.217%
26	13.198	1887	1889	1891	rBV3	7475	7900	2.52%	0.342%
27	13.221	1891	1893	1895	rVB3	7359	5168	1.65%	0.224%
28	13.321	1908	1910	1911	rBV2	8389	6230	1.99%	0.270%
29	13.357	1914	1916	1917	rBV2	7290	5031	1.60%	0.218%
30	13.398	1921	1923	1925	rBV3	5932	5485	1.75%	0.238%
31	13.451	1929	1932	1934	rBV4	18477	15891	5.07%	0.689%
32	13.486	1936	1938	1939	rBV2	6543	5104	1.63%	0.221%
33	13.510	1939	1942	1944	rVB4	8673	7841	2.50%	0.340%
34	13.533	1944	1946	1948	rBV3	12423	11857	3.78%	0.514%
35	13.580	1953	1954	1958	rBV3	7809	10930	3.49%	0.474%
36	13.780	1986	1988	1989	rVB2	11213	4909	1.57%	0.213%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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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37	13.945	2014	2016	2019	rBV4	9238	11257	3.59%	0.488%
38	14.033	2026	2031	2035	rBV	262210	278861	88.92%	12.088%
39	14.168	2053	2054	2055	rBV	19225	9405	3.00%	0.408%
40	14.545	2116	2118	2119	rBV2	15552	6307	2.01%	0.273%
41	15.445	2268	2271	2273	rBV4	24019	31696	10.11%	1.374%
42	15.515	2279	2283	2292	rVB	151733	204944	65.35%	8.884%
43	16.474	2444	2446	2447	rBV2	13409	9375	2.99%	0.406%
44	17.445	2609	2611	2613	rBV3	12701	10376	3.31%	0.450%
45	18.092	2719	2721	2724	rBV4	12331	13372	4.26%	0.580%
46	18.145	2728	2730	2731	rBV2	12894	10676	3.40%	0.463%
47	18.180	2735	2736	2737	rBV	13561	6144	1.96%	0.266%
48	18.886	2854	2856	2858	rBV3	12799	8999	2.87%	0.390%

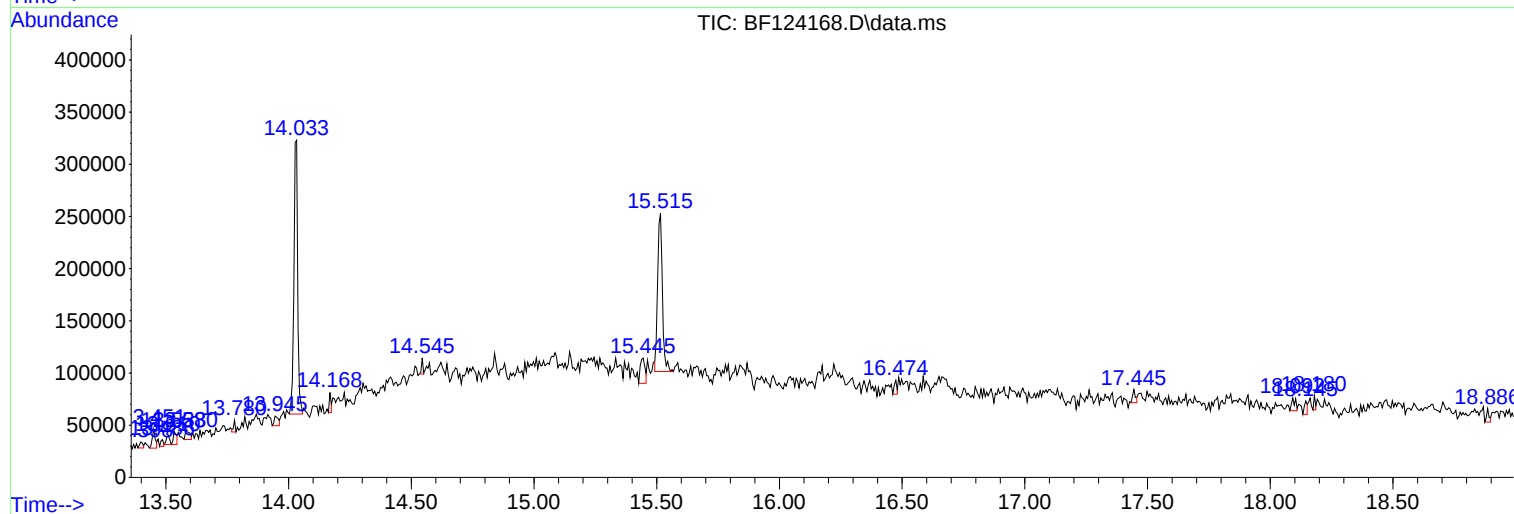
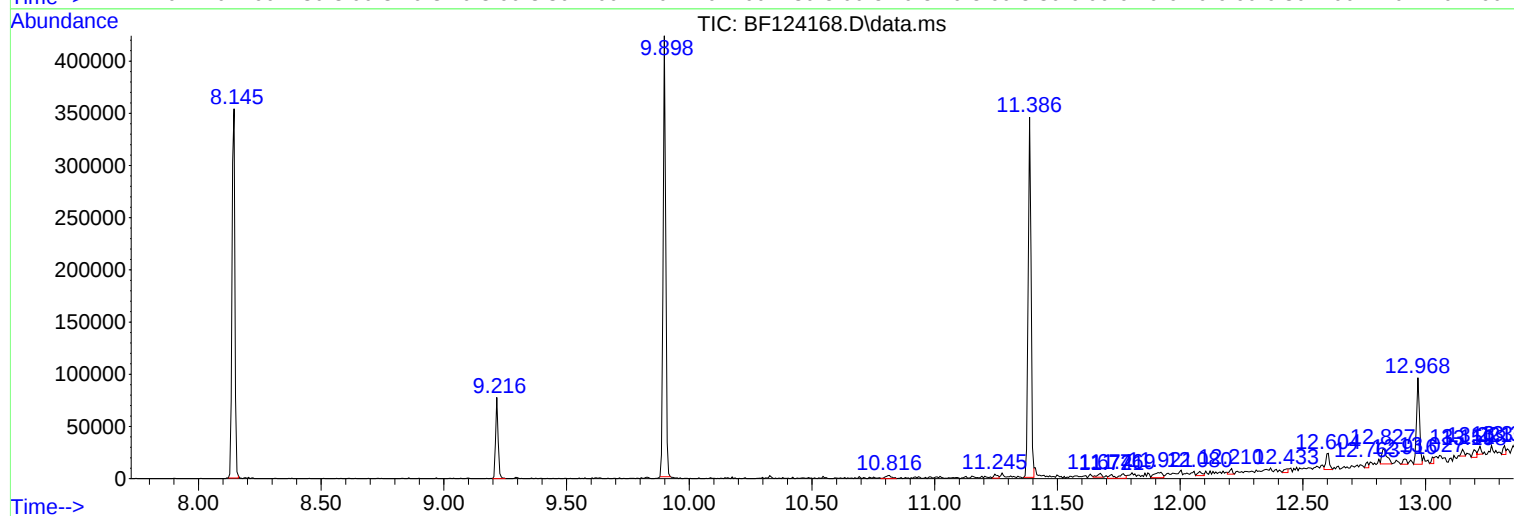
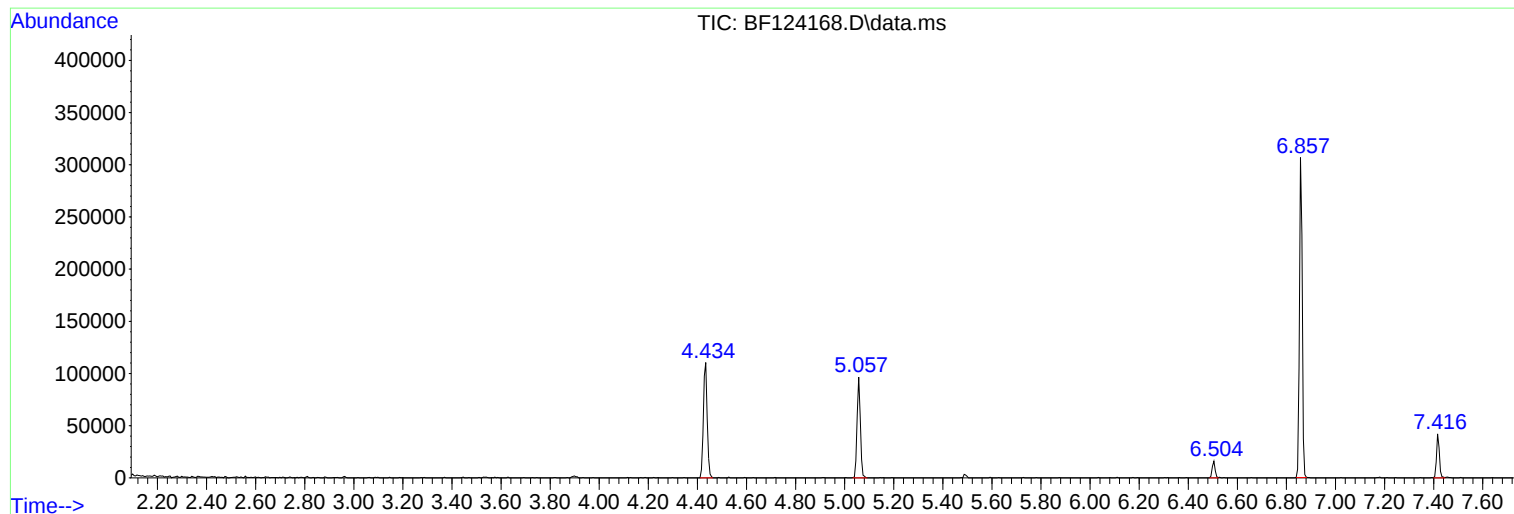
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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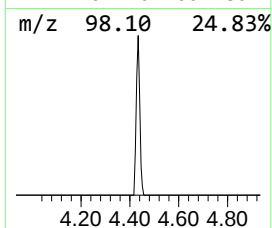
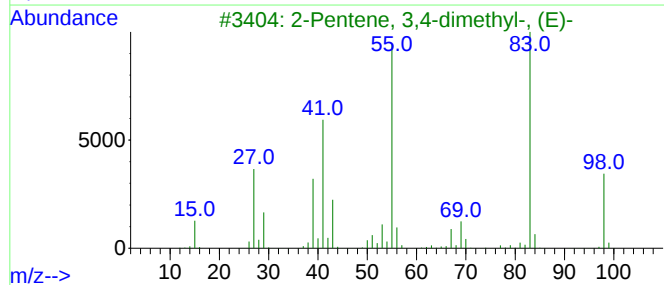
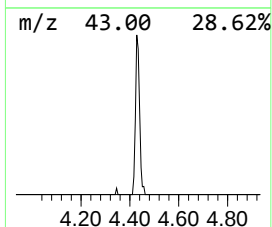
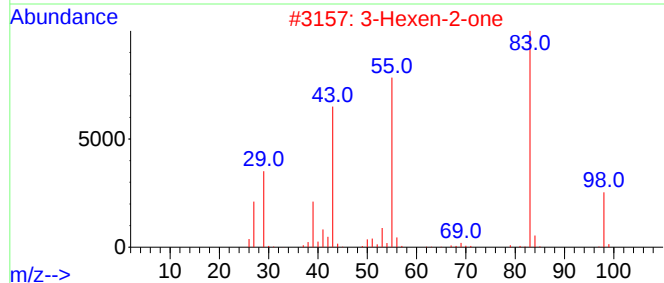
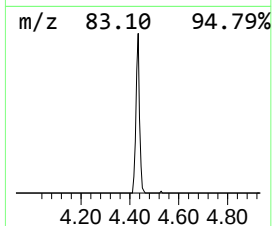
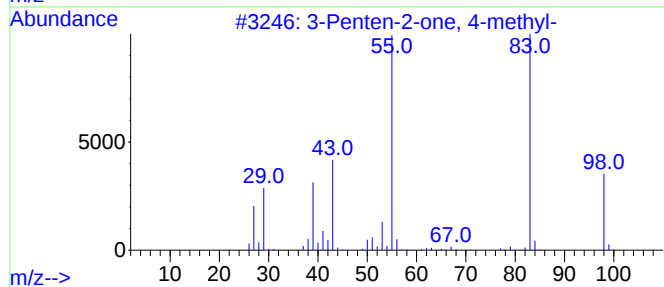
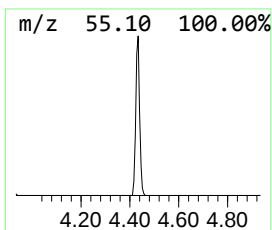
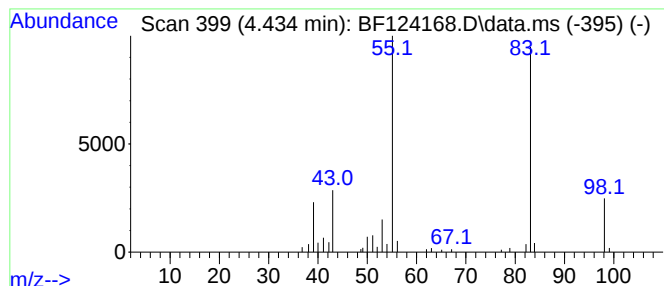
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	9.74 ng	118867	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4		1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	72
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



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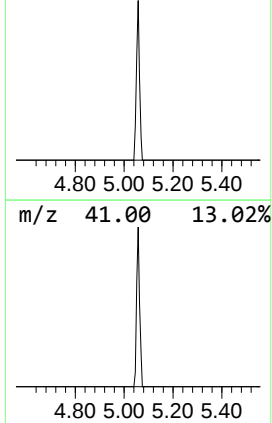
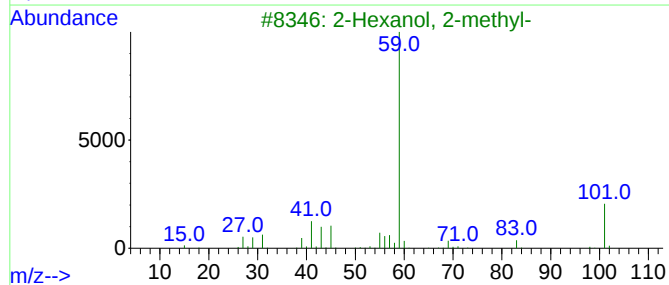
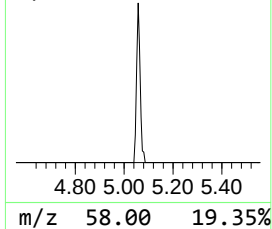
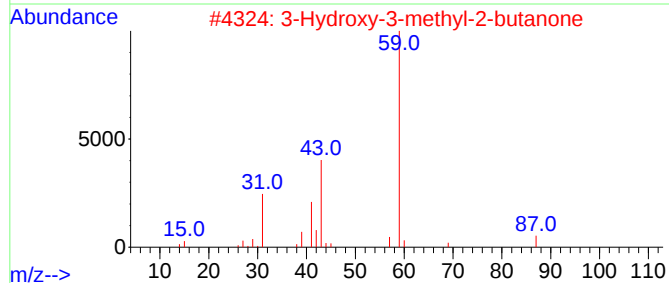
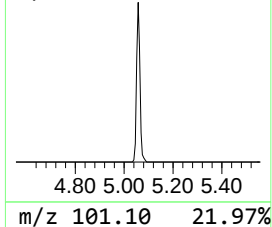
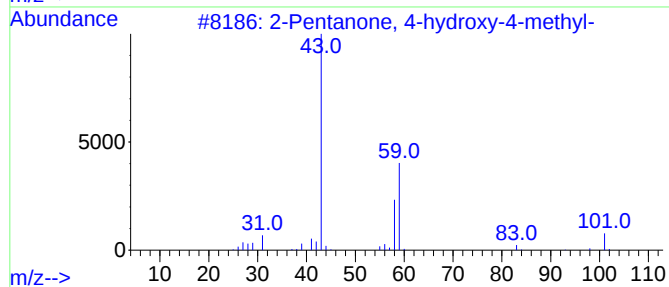
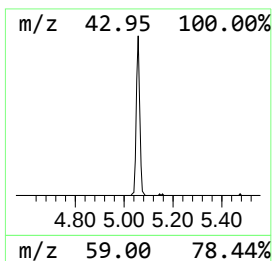
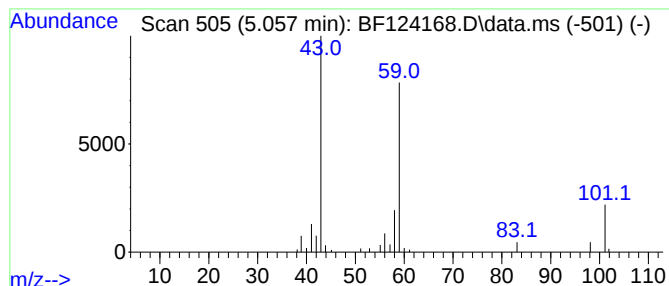
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	7.44 ng	90817	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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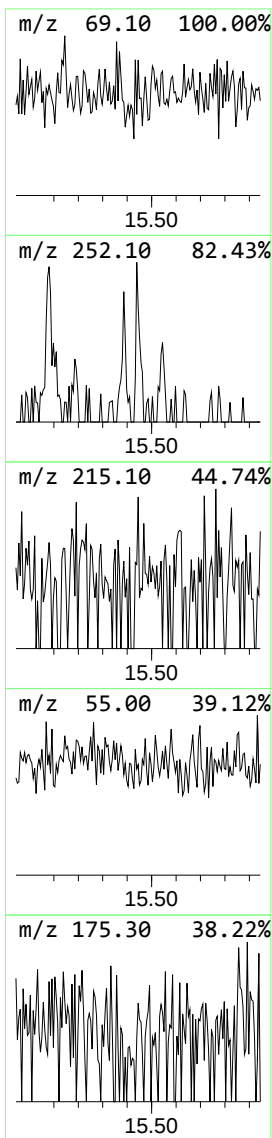
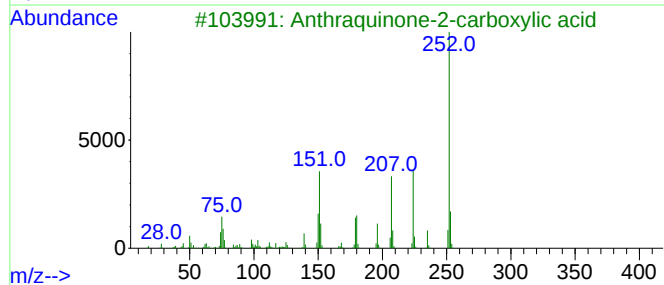
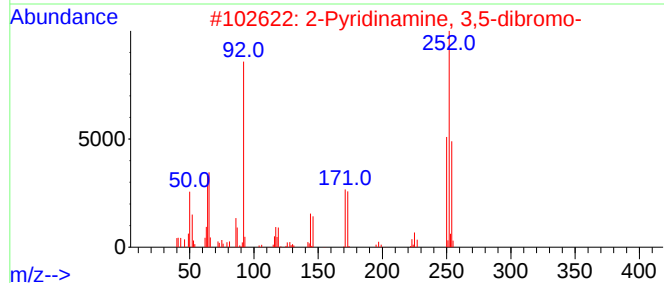
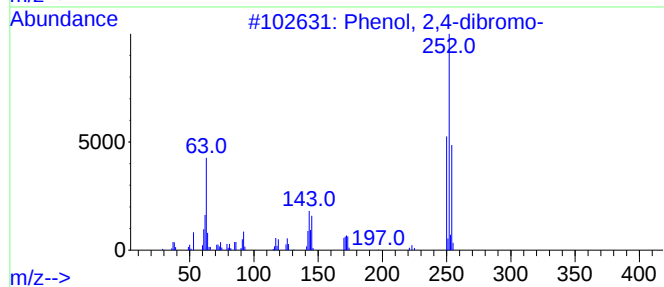
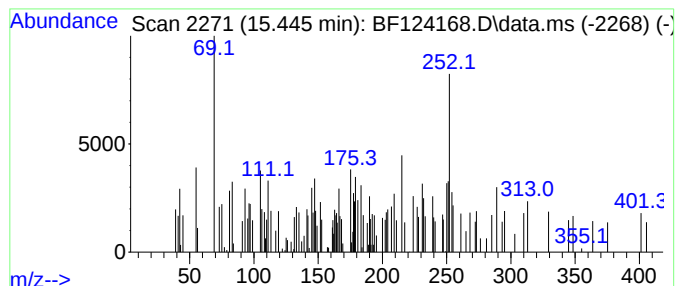
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.445 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	3.09 ng	31696	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	38
2			2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	38
3			Anthraquinone-2-carboxylic acid	252	C15H8O4	000117-78-2	35
4			Phenyl-(5-phenylthiazol-2-yl)-amine	252	C15H12N2S	306321-46-0	35
5			2-[2',4'-Dichlorophenyl]-7-methy...	287	C16H11Cl2N	1000253-84-3	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.434	9.7	ng	118867	1	6.857	244192	20.0
2-Pentanone, 4-...	5.057	7.4	ng	90817	1	6.857	244192	20.0
unknown15.445	15.445	3.1	ng	31696	6	15.515	204944	20.0