

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111617\
 Data File : BF100626.D
 Acq On : 16 Nov 2017 13:16
 Operator : SJ/JU
 Sample : I6302-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-04-111317-A

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.128	511	517	528	rVB	823388	1132918	30.21%	3.840%
2	5.516	577	583	586	rBV	2562421	2700572	72.01%	9.154%
3	6.510	746	752	755	rBV	2346803	2397407	63.92%	8.126%
4	6.657	771	777	780	rBV	2744157	2975937	79.35%	10.087%
5	6.881	812	815	819	rVB	788415	640014	17.07%	2.169%
6	7.039	838	842	845	rBV	2658236	2390768	63.75%	8.104%
7	7.445	905	911	914	rBV	2006012	2007719	53.53%	6.805%
8	8.163	1028	1033	1035	rBV	986674	891392	23.77%	3.021%
9	8.181	1035	1036	1043	rVB	108090	75492	2.01%	0.256%
10	9.239	1210	1216	1219	rBV	3463913	3567288	95.12%	12.091%
11	9.916	1323	1331	1334	rBV2	1092364	974882	25.99%	3.304%
12	9.945	1334	1336	1339	rVB	59329	45856	1.22%	0.155%
13	10.463	1420	1424	1427	rBV	59005	48367	1.29%	0.164%
14	10.710	1460	1466	1469	rBV	2036790	2269535	60.51%	7.693%
15	11.404	1579	1584	1586	rBV	1140498	1046283	27.90%	3.546%
16	11.421	1586	1587	1591	rVB	100073	69415	1.85%	0.235%
17	11.627	1616	1622	1626	rBV	66213	54950	1.47%	0.186%
18	12.733	1806	1810	1813	rBV	719518	588113	15.68%	1.993%
19	12.992	1848	1854	1857	rBV	3452473	3750423	100.00%	12.712%
20	13.145	1875	1880	1885	rBV	175899	159151	4.24%	0.539%
21	13.486	1935	1938	1943	rBV	124440	114266	3.05%	0.387%
22	14.039	2028	2032	2035	rVB	1004286	913372	24.35%	3.096%
23	15.509	2277	2282	2291	rBV2	530172	688680	18.36%	2.334%

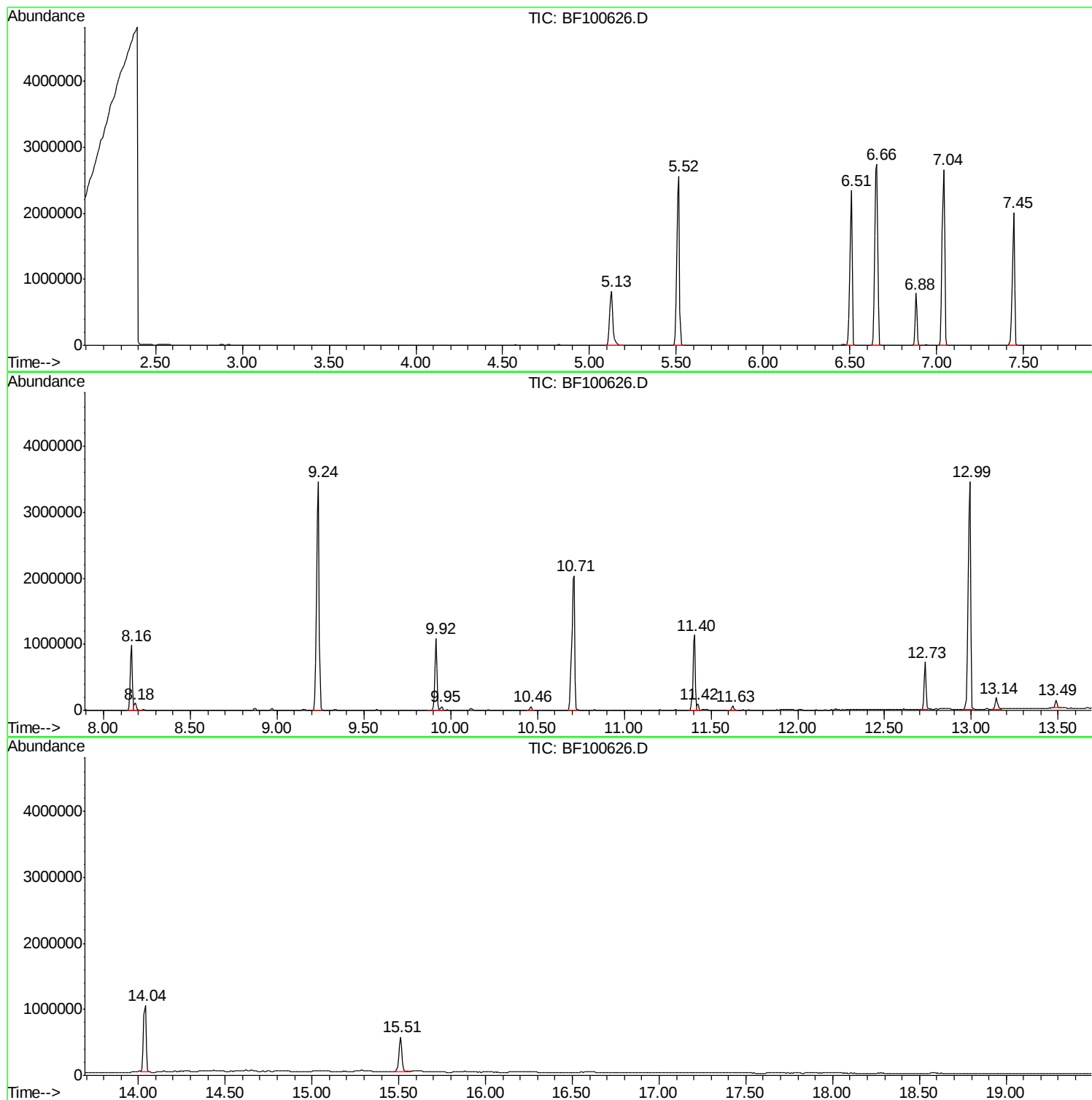
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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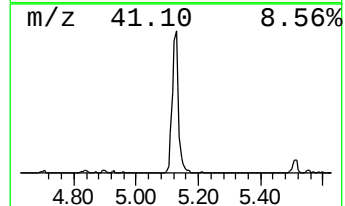
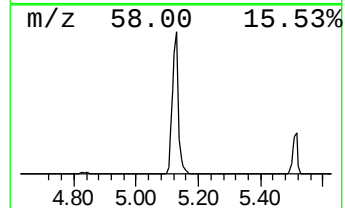
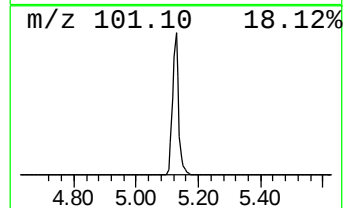
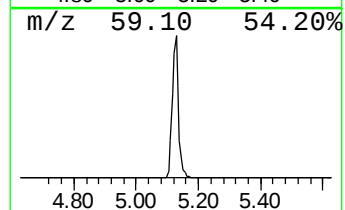
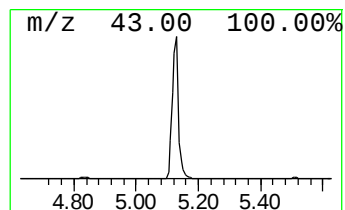
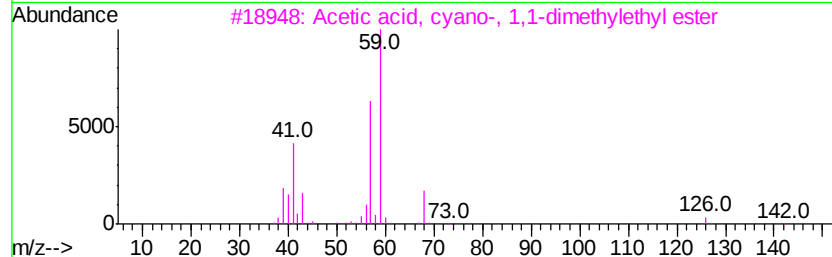
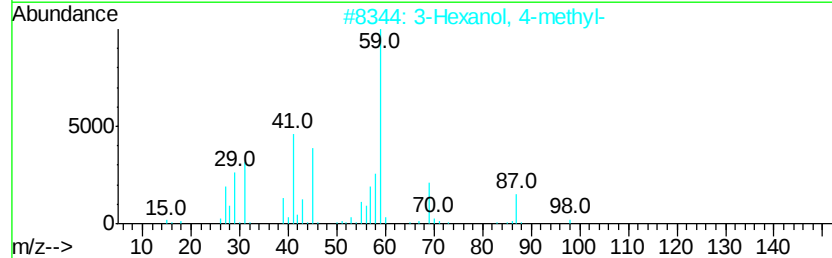
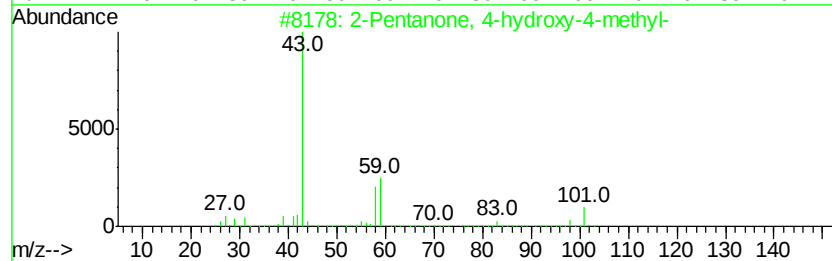
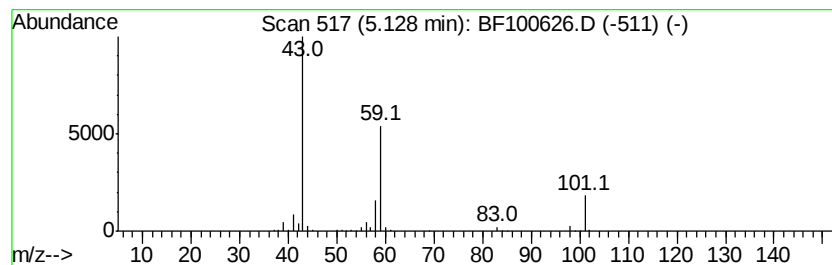
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	35.40 ng	1132920	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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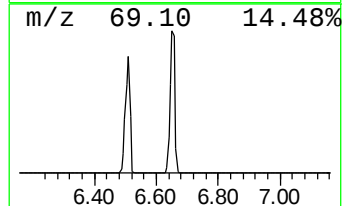
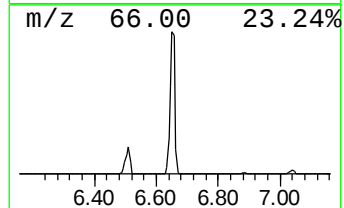
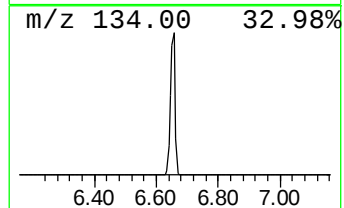
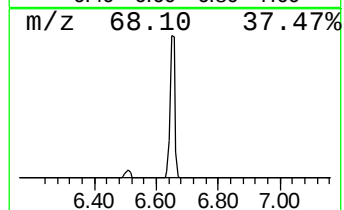
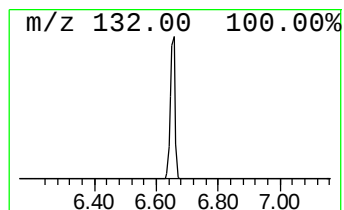
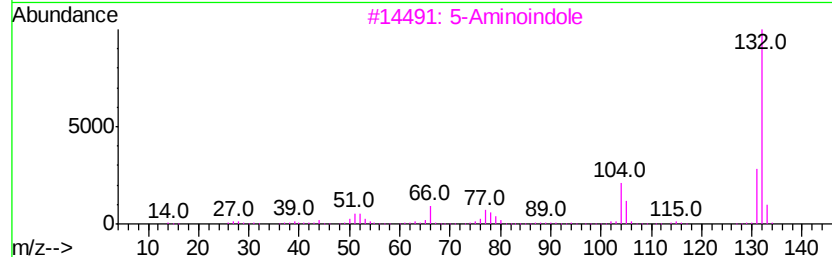
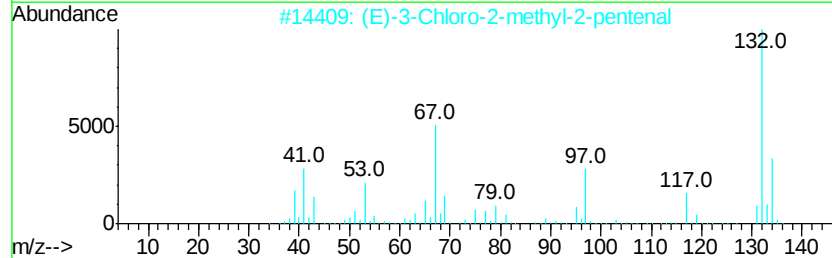
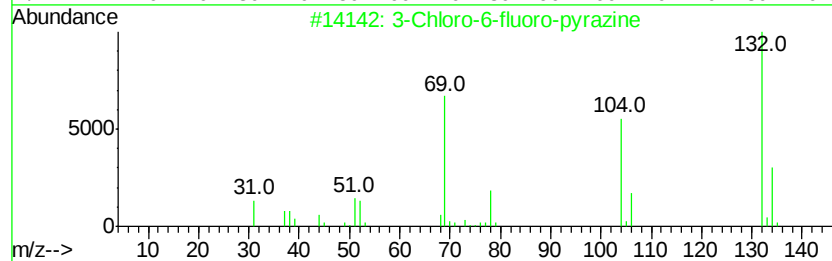
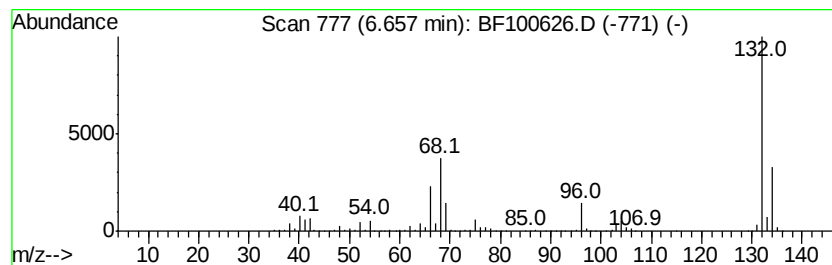
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	93.00 ng	2975940	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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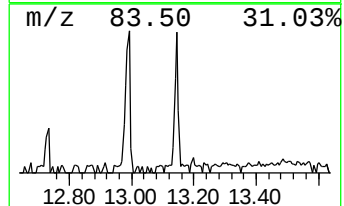
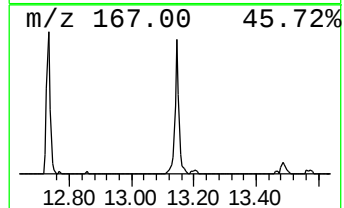
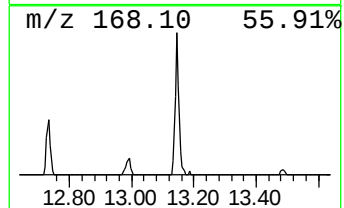
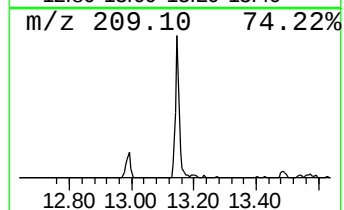
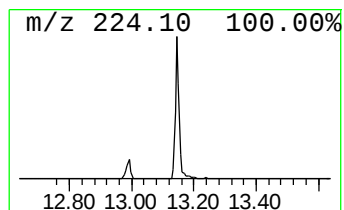
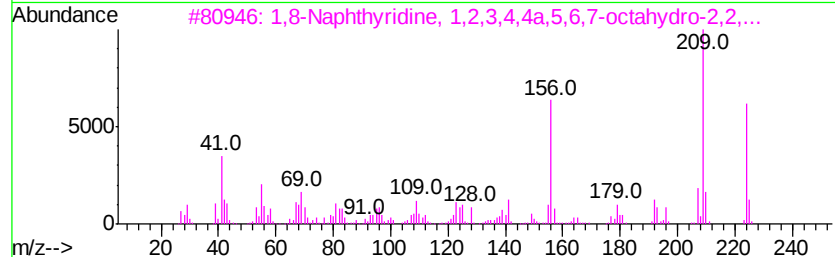
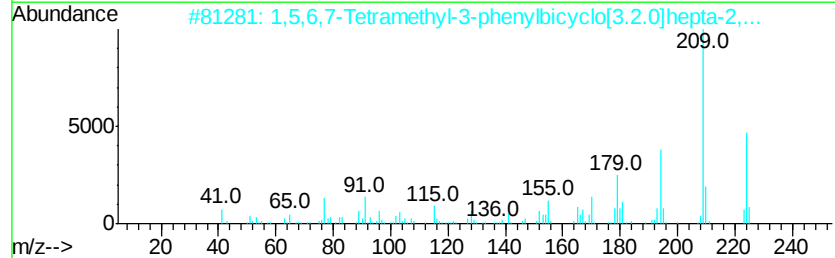
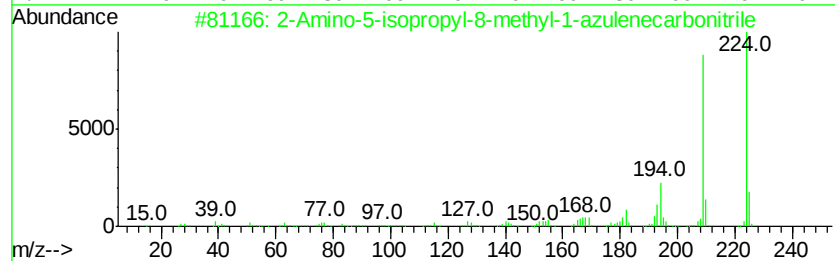
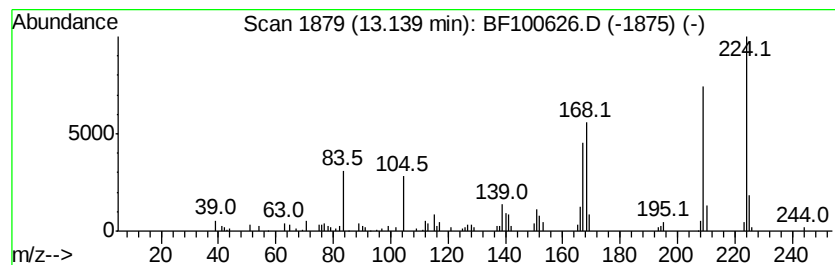
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Peak Number 4 2-Amino-5-isopropyl-8-methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	3.48 ng	159151	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Amino-5-isopropyl-8-methyl-1-a...	224	C15H16N2	093946-48-6	52
2		1,5,6,7-Tetramethyl-3-phenylbicy...	224	C17H20	126584-00-7	49
3		1,8-Naphthyridine, 1,2,3,4,4a,5,...	224	C13H24N2O	069340-71-2	47
4		Benzoic acid, 3-[(trimethylsilyl...	224	C11H16O3Si	027798-50-1	47
5		2,3,4,6-Tetramethoxystyrene	224	C12H16O4	048153-74-8	47



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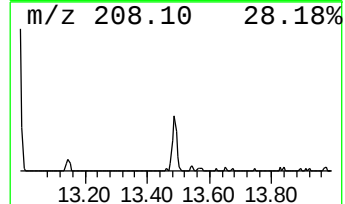
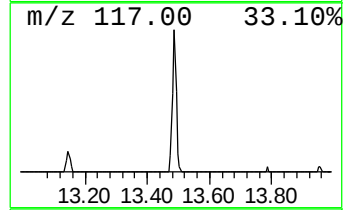
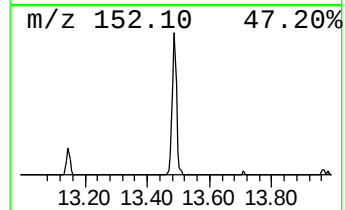
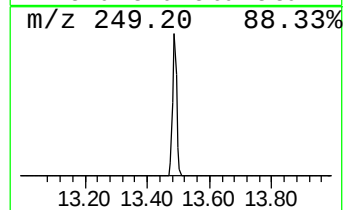
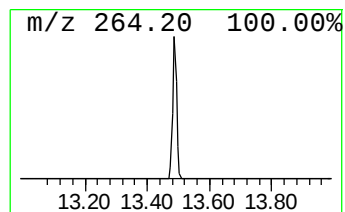
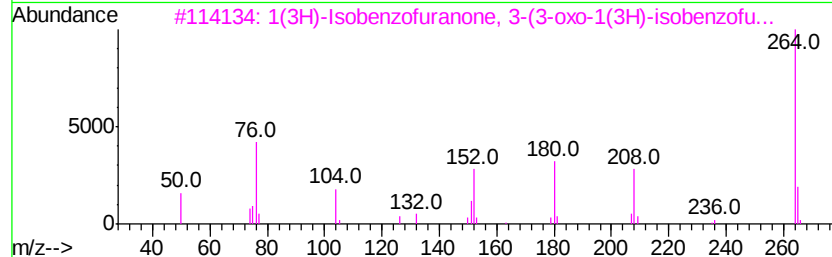
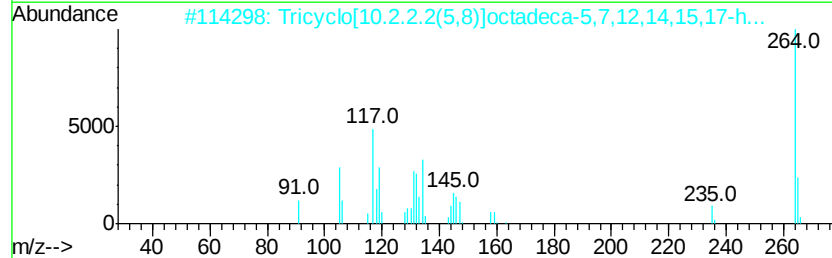
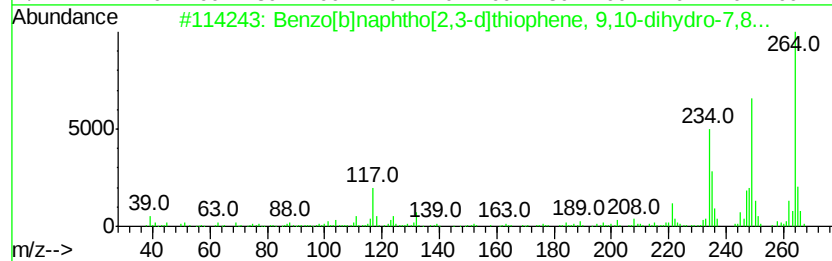
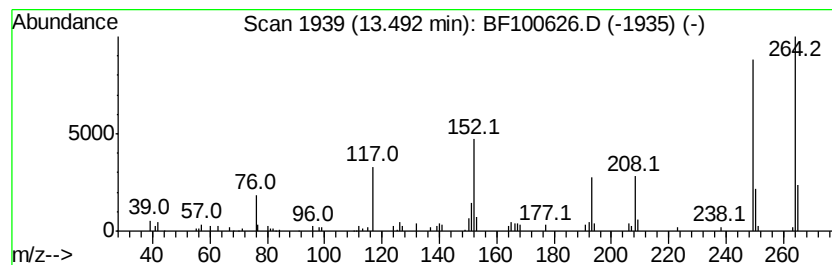
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Peak Number 5 unknown13.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.50 ng	114266	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]naphtho[2,3-d]thiophene,...	264	C18H16S	024964-00-9	37
2		Tricyclo[10.2.2.2(5,8)]octadeca-...	264	C20H24	024777-38-6	35
3		1(3H)-Isobenzofuranone, 3-(3-oxo...	264	C16H8O4	000482-23-5	35
4		Anthraquinone, 2,3,6,7-tetramethyl-	264	C18H16O2	015247-68-4	27
5		Chromeno(4,3-c)chromene-5,11-dione	264	C16H8O4	013225-81-5	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	35.4	ng	1132920	1	6.88	640014	20.0
unknown6.66	6.66	93.0	ng	2975940	1	6.88	640014	20.0
2-Amino-5-isoprop...	13.14	3.5	ng	159151	5	14.04	913372	20.0
unknown13.49	13.49	2.5	ng	114266	5	14.04	913372	20.0