

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
 Data File : BF085122.D
 Acq On : 2 Mar 2016 16:33
 Operator : SJ/IZ
 Sample : H1620-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-05

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % 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:\HPCHEM1\BNA_F\METHODS\8270-BF030116.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	5.190	251	254	257	rBV	323868	334458	6.04%	0.875%
2	5.590	287	289	292	rBV	1825030	2022631	36.53%	5.293%
3	6.607	375	378	380	rBV	1702956	1401915	25.32%	3.669%
4	6.756	388	391	394	rBV	3889217	3681520	66.50%	9.635%
5	6.996	409	412	414	rBV	923875	1097512	19.82%	2.872%
6	7.144	423	425	428	rVB	3005160	3661643	66.14%	9.583%
7	7.556	458	461	463	rBV	3353816	3417987	61.74%	8.945%
8	8.276	521	524	526	rBV	1843598	1517742	27.41%	3.972%
9	9.350	615	618	621	rBV	4587722	5536300	100.00%	14.489%
10	9.739	650	652	654	rVB	590404	541349	9.78%	1.417%
11	10.036	675	678	680	rBV	1678413	1642695	29.67%	4.299%
12	10.459	711	715	716	rBV3	42635	69417	1.25%	0.182%
13	10.825	744	747	749	rBV	3611445	3866510	69.84%	10.119%
14	10.951	754	758	759	rBV2	33348	67189	1.21%	0.176%
15	11.522	805	808	810	rBV	1383422	1485518	26.83%	3.888%
16	12.036	851	853	855	rBV	124849	141212	2.55%	0.370%
17	12.745	913	915	919	rVB2	50015	63944	1.15%	0.167%
18	12.825	920	922	924	rBV	92241	98625	1.78%	0.258%
19	13.099	944	946	949	rBV	3410238	4367291	78.88%	11.430%
20	13.625	990	992	994	rBV	96456	103255	1.87%	0.270%
21	13.945	1018	1020	1022	rVB2	61442	66379	1.20%	0.174%
22	13.991	1022	1024	1028	rBV3	53957	96689	1.75%	0.253%
23	14.059	1028	1030	1032	rVV	62554	74074	1.34%	0.194%
24	14.151	1036	1038	1041	rBV	1042358	1012225	18.28%	2.649%
25	14.528	1069	1071	1075	rBV	64932	148976	2.69%	0.390%
26	14.597	1075	1077	1079	rBV	60050	57893	1.05%	0.152%
27	14.665	1081	1083	1087	rBV2	83013	135007	2.44%	0.353%
28	14.917	1103	1105	1108	rVB	97470	116399	2.10%	0.305%
29	14.985	1109	1111	1114	rBV	63129	84633	1.53%	0.221%
30	15.637	1165	1168	1177	rVB	856454	1299236	23.47%	3.400%

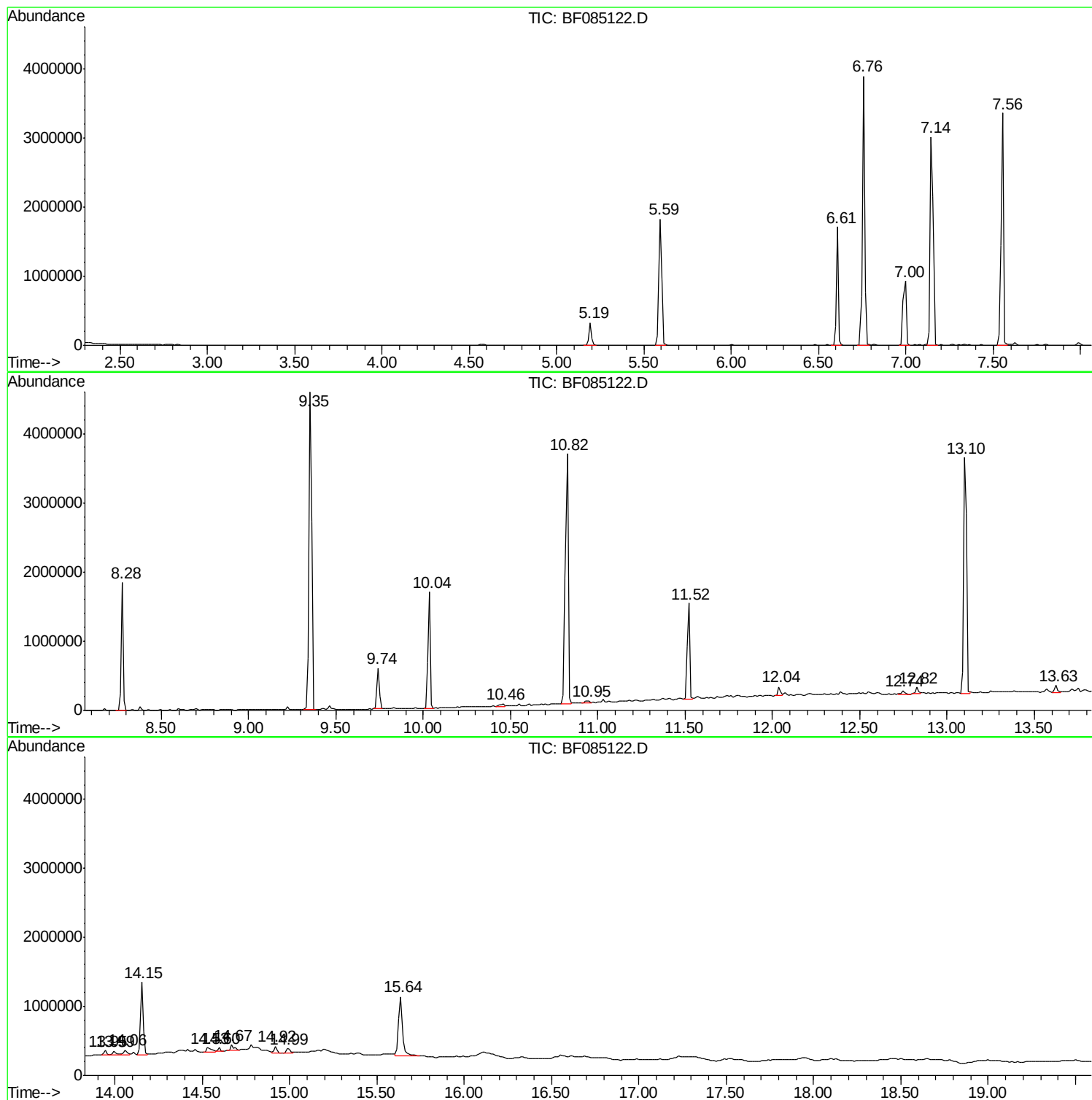
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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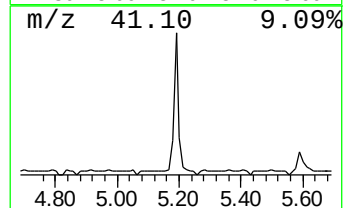
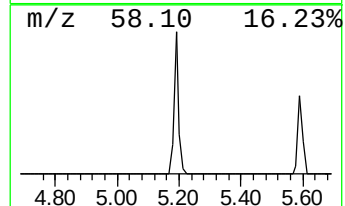
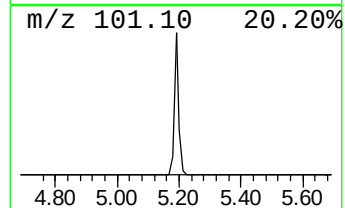
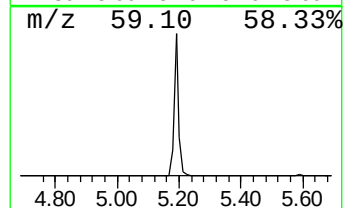
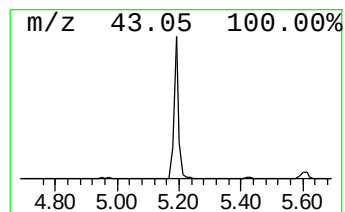
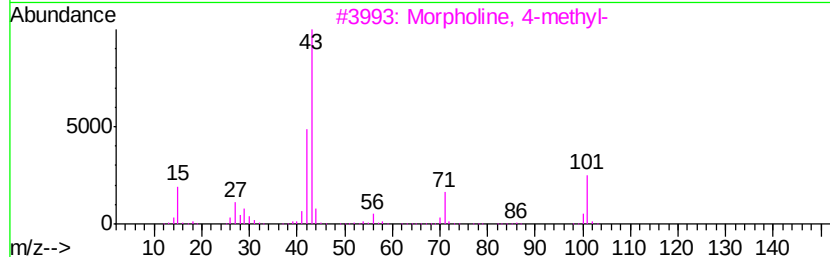
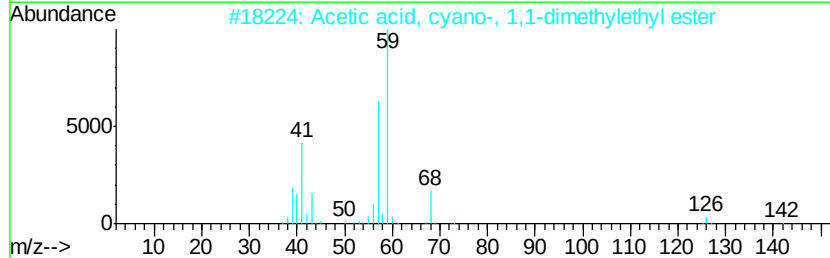
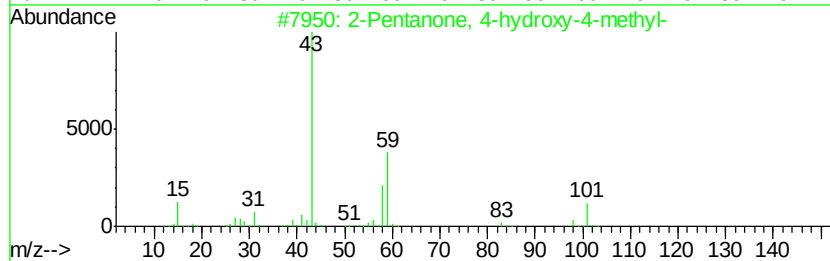
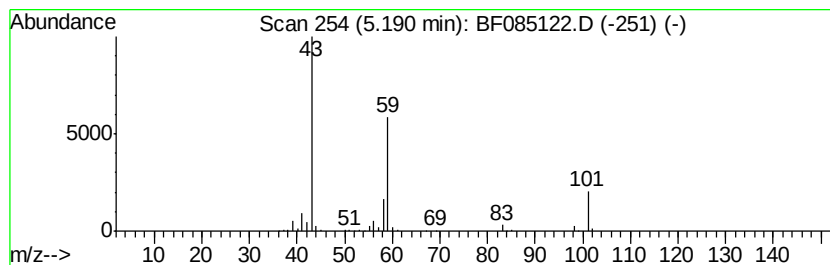
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.19	6.09 ng	334458	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane	58	C4H10	000106-97-8	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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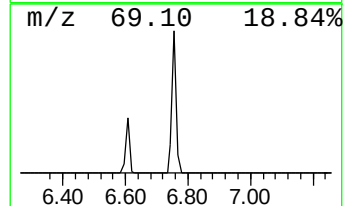
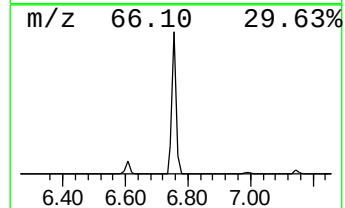
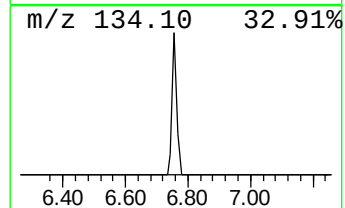
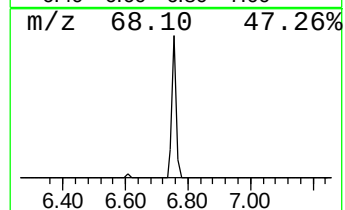
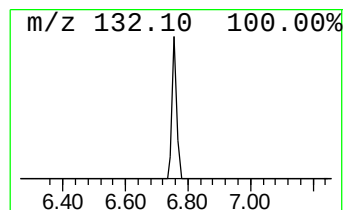
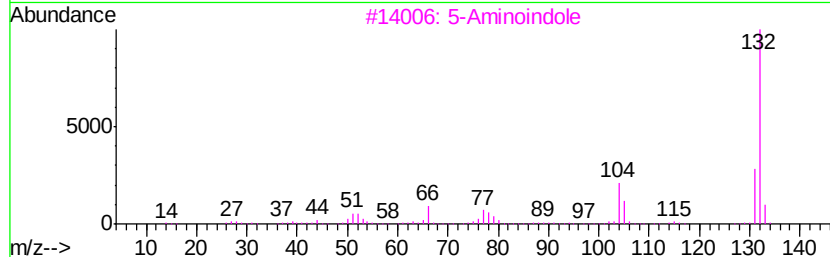
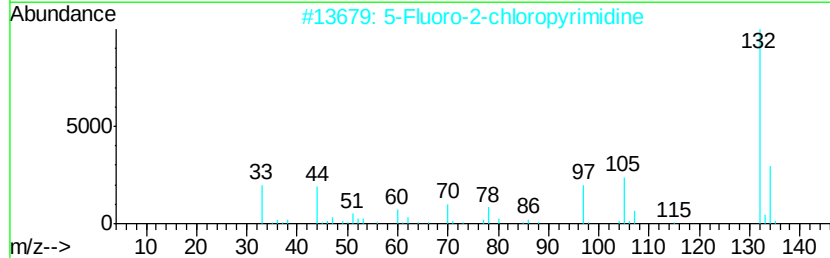
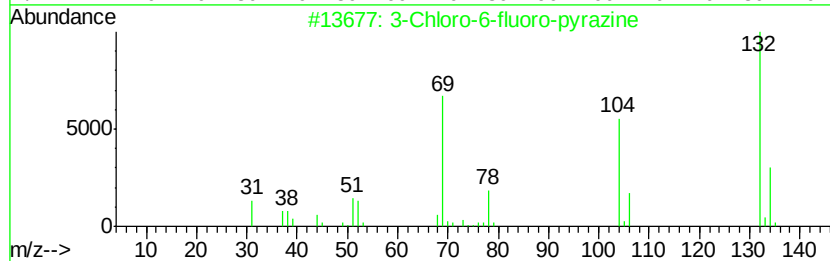
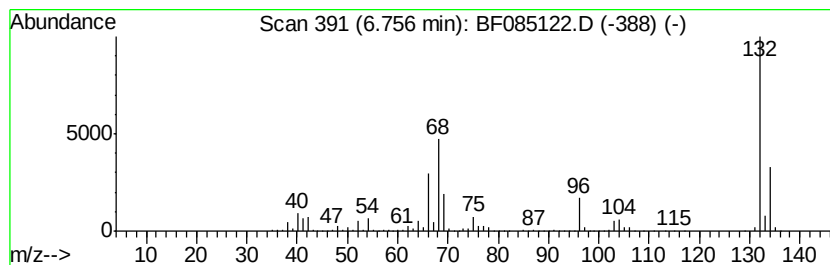
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Peak Number 2 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	67.09 ng	3681520	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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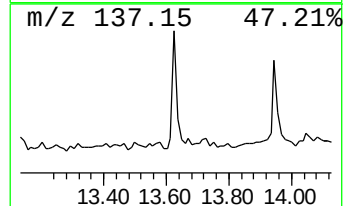
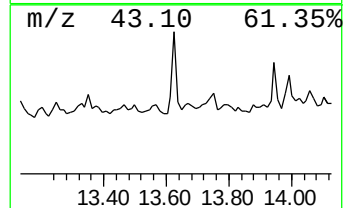
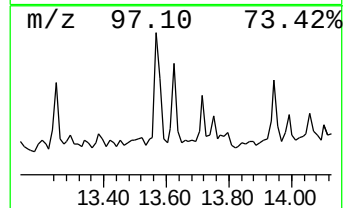
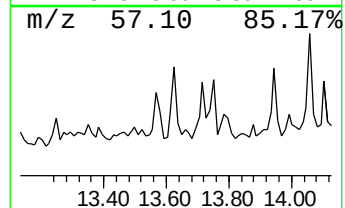
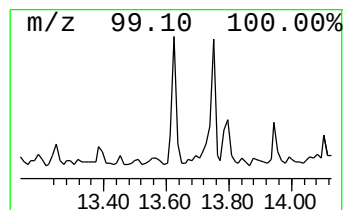
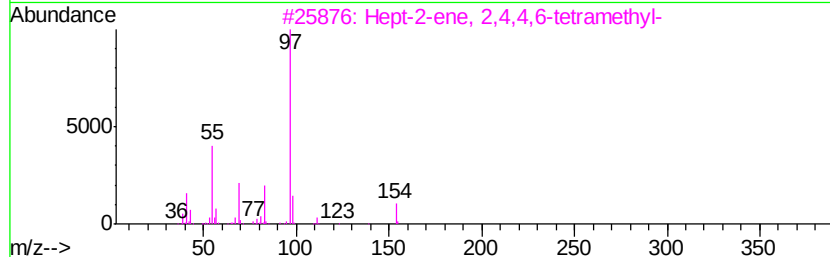
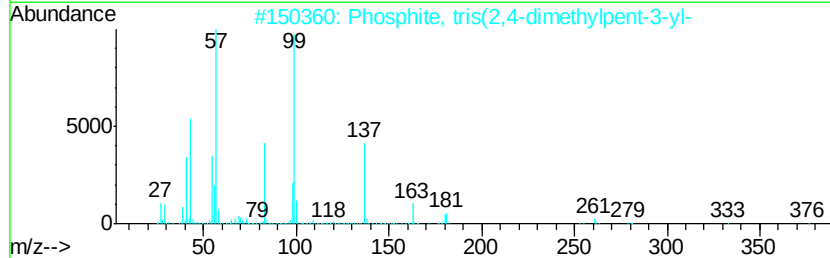
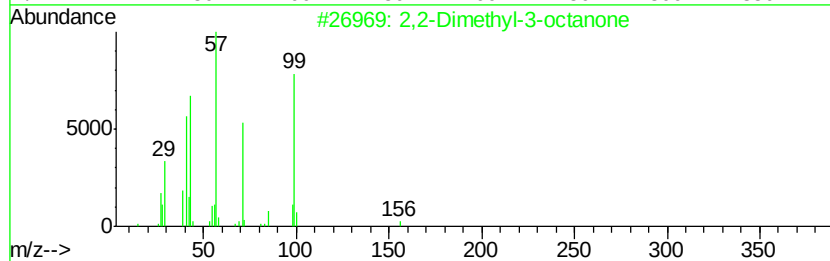
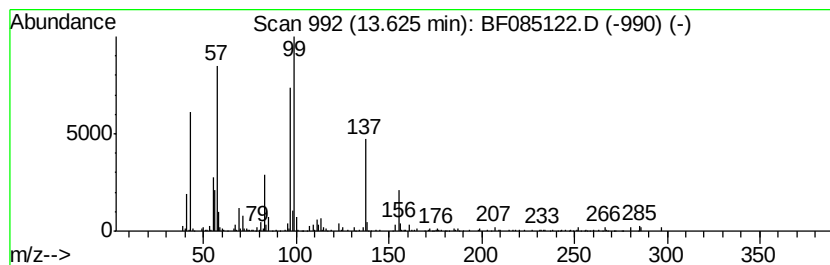
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Peak Number 4 unknown13.63 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.04 ng	103255	Chrysene-d12	14.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-3-octanone			156	C10H20O	005340-64-7	30
2	Phosphite, tris(2,4-dimethylpent...			376	C21H45O3P	1000159-84-4	25
3	Hept-2-ene, 2,4,4,6-tetramethyl-			154	C11H22	103982-58-7	22
4	4H-Imidazol-4-one, 2-amino-1,5-d...			99	C3H5N3O	000503-86-6	22
5	4-Piperidinone			99	C5H9NO	041661-47-6	22



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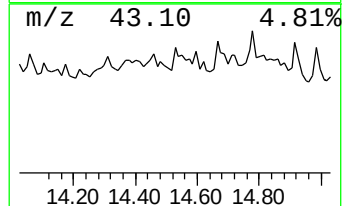
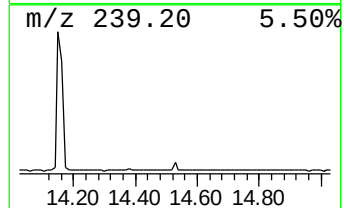
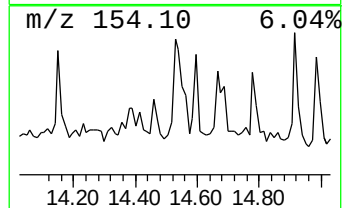
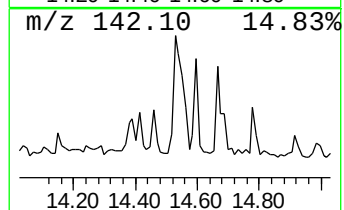
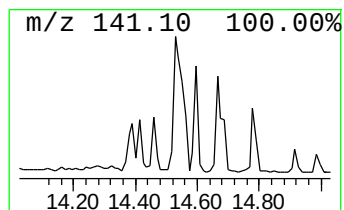
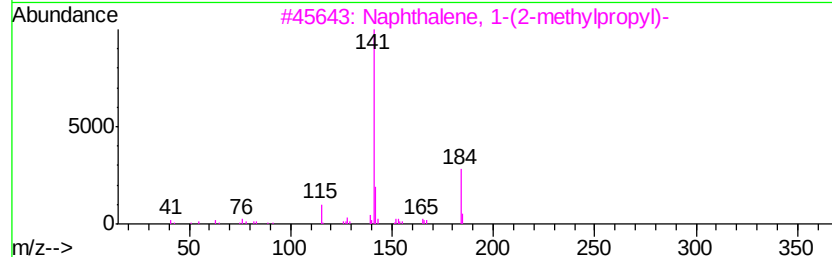
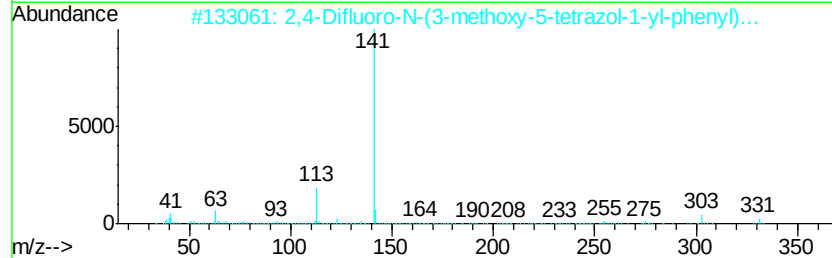
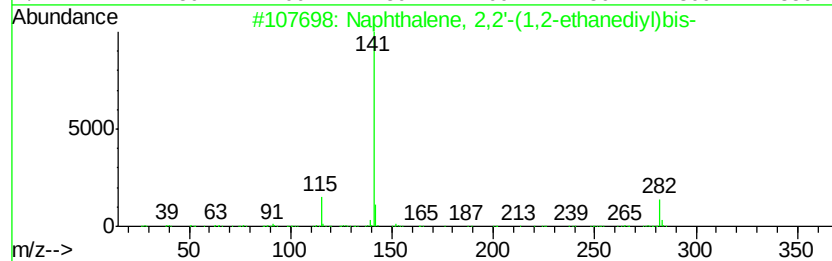
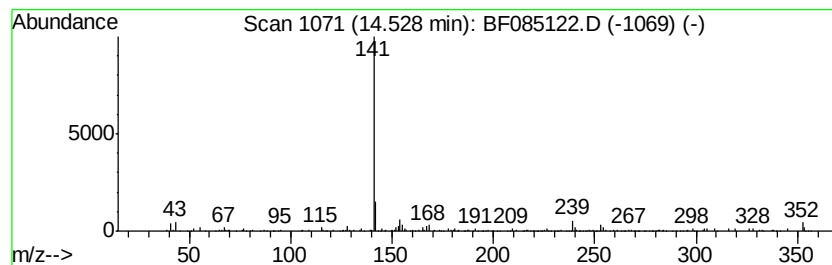
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Peak Number 5 Naphthalene, 2,2'-(1,2-etha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.94 ng	148976	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,2'-(1,2-ethanediy...	282	C22H18	021969-45-9	64
2		2,4-Difluoro-N-(3-methoxy-5-tetr...	331	C15H11F2N5O2	1000295-28-9	39
3		Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	39
4		Piperidin-4-ol, 1,2,5-trimethyl-...	283	C19H25NO	329789-67-5	39
5		Pyrazol-4-amine, 3,5-dimethyl-1-...	251	C16H17N3	1000273-77-6	39



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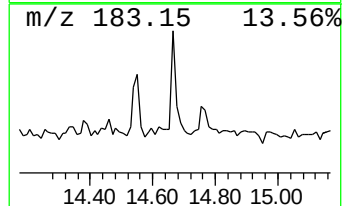
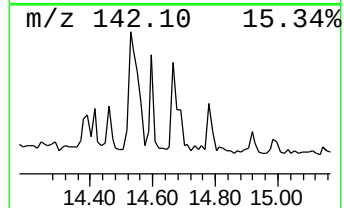
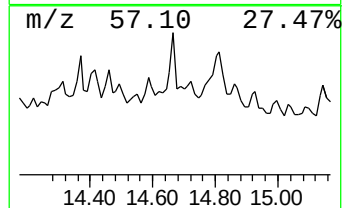
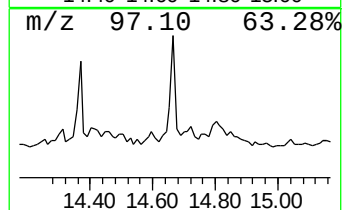
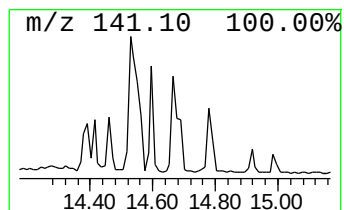
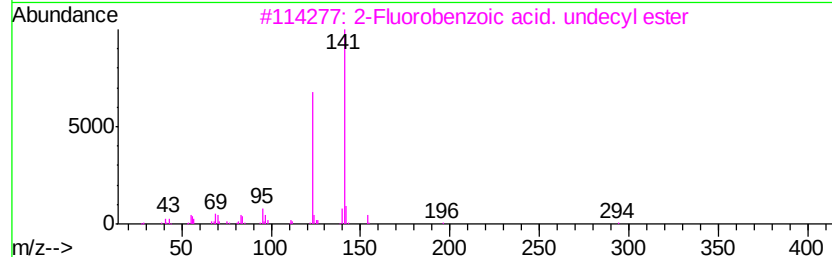
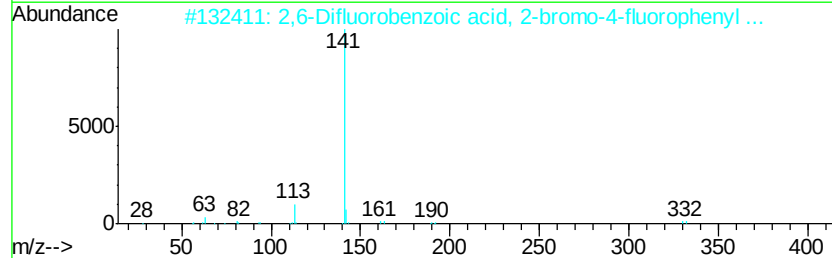
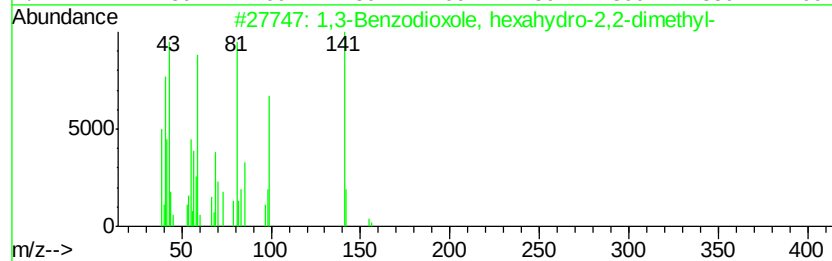
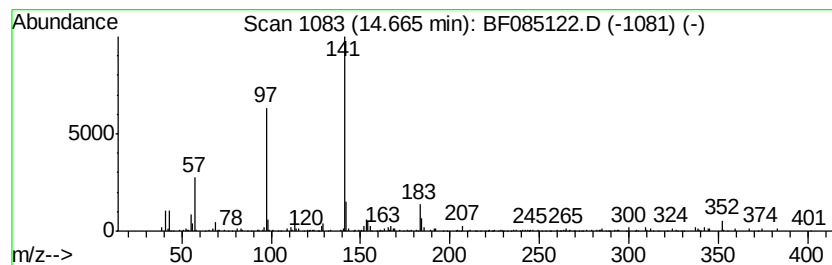
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Peak Number 6 1,3-Benzodioxole, hexahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.67 ng	135007	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzodioxole, hexahydro-2,2-...	156	C9H16O2	005664-14-2	53
2		2,6-Difluorobenzoic acid, 2-brom...	330	C13H6BrF3O2	1000292-62-5	47
3		2-Fluorobenzoic acid, undecyl ester	294	C18H27FO2	1000282-96-3	46
4		Cyclohexanone, 5-methyl-2-(1-met...	183	C11H21NO	057396-81-3	40
5		Naphthalene, 1,1'-(1,2-ethanedi...	282	C22H18	015374-45-5	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	6.1	ng	334458	1	7.00	1097510	20.0
unknown6.76	6.76	67.1	ng	3681520	1	7.00	1097510	20.0
unknown13.63	13.63	2.0	ng	103255	5	14.15	1012230	20.0
Naphthalene, 2,2'...	14.53	2.9	ng	148976	5	14.15	1012230	20.0
1,3-Benzodioxole,...	14.67	2.7	ng	135007	5	14.15	1012230	20.0