

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061116\
Data File : BF087925.D
Acq On : 12 Jun 2016 3:24
Operator : UM/SJ
Sample : PB91213BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB91213BL

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-BF060716.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	1.678	3	8	11	rVB	2989855	3992815	100.00%	12.724%
2	1.735	11	13	22	rVV	456405	975360	24.43%	3.108%
3	1.861	22	24	41	rVB	1551688	2710645	67.89%	8.638%
4	4.981	294	297	302	rBV	114533	155667	3.90%	0.496%
5	5.393	330	333	336	rBV	1778915	2293399	57.44%	7.309%
6	6.433	421	424	427	rBV	1923469	2090963	52.37%	6.664%
7	6.570	433	436	438	rBV	2205374	2565164	64.24%	8.175%
8	6.799	453	456	458	rBV	750636	617490	15.47%	1.968%
9	6.959	467	470	472	rBV	2070338	2061358	51.63%	6.569%
10	7.370	502	506	508	rBV	1221912	1671844	41.87%	5.328%
11	8.090	566	569	571	rBV	798671	858138	21.49%	2.735%
12	9.165	660	663	666	rBV	2549024	2848211	71.33%	9.077%
13	9.839	719	722	725	rBV	1026730	959012	24.02%	3.056%
14	10.628	788	791	794	rBV	1639462	1741644	43.62%	5.550%
15	11.325	849	852	854	rBV	1002713	1060986	26.57%	3.381%
16	12.742	974	976	978	rBV	136411	128104	3.21%	0.408%
17	12.914	988	991	993	rBV	2843273	2926853	73.30%	9.327%
18	13.439	1035	1037	1039	rBV	70397	83782	2.10%	0.267%
19	13.954	1079	1082	1084	rBV	1049989	946965	23.72%	3.018%
20	15.371	1203	1206	1208	rBV	470803	690890	17.30%	2.202%

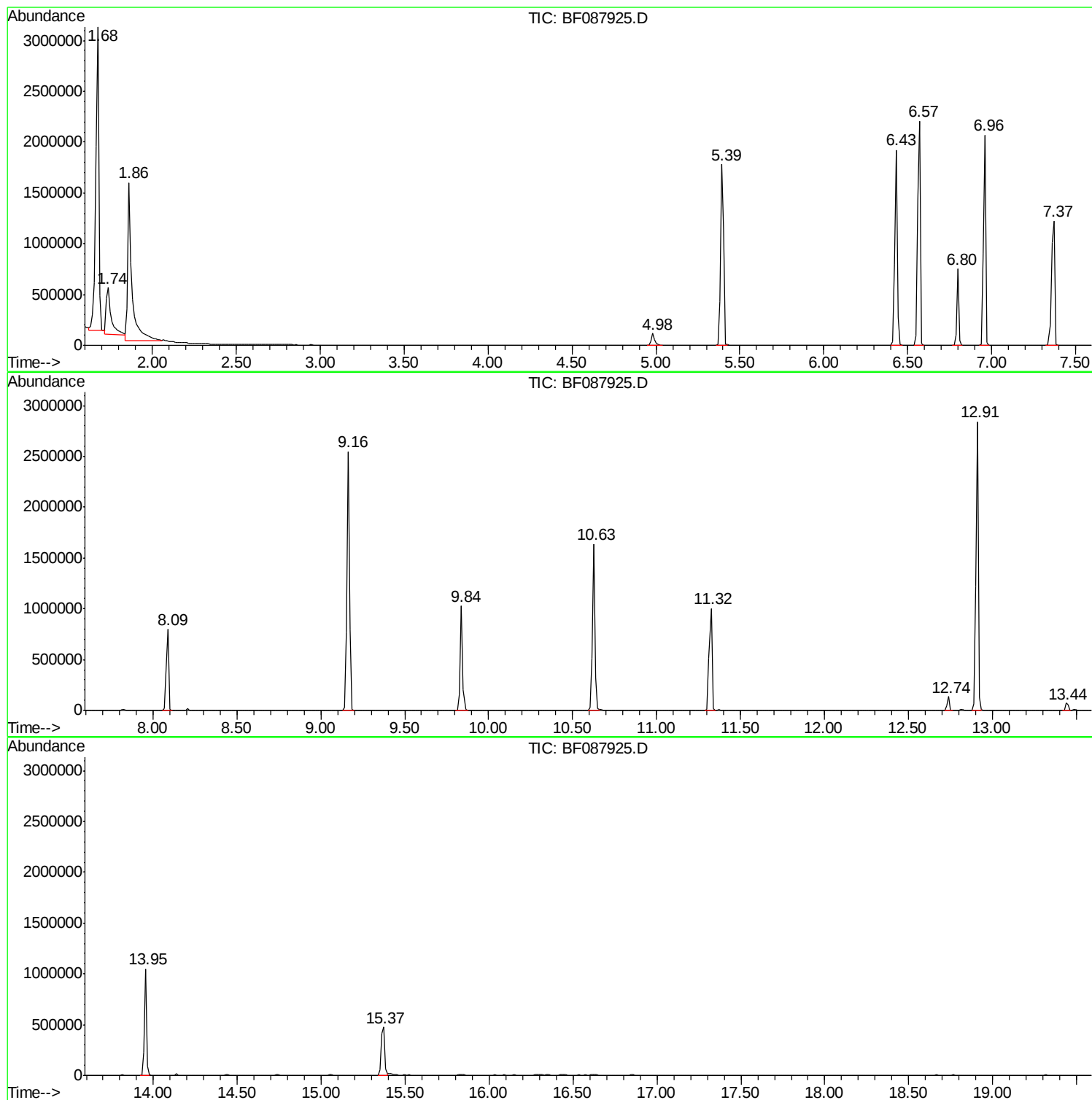
Sum of corrected areas: 31379290

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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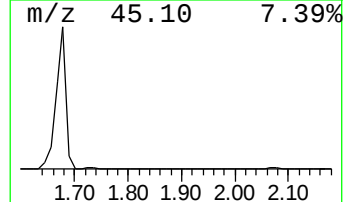
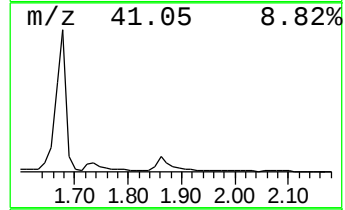
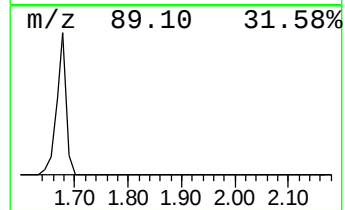
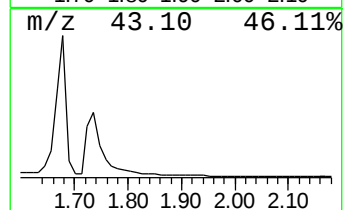
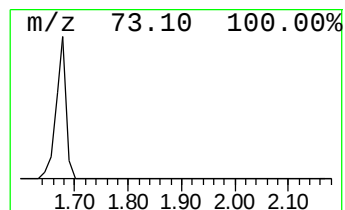
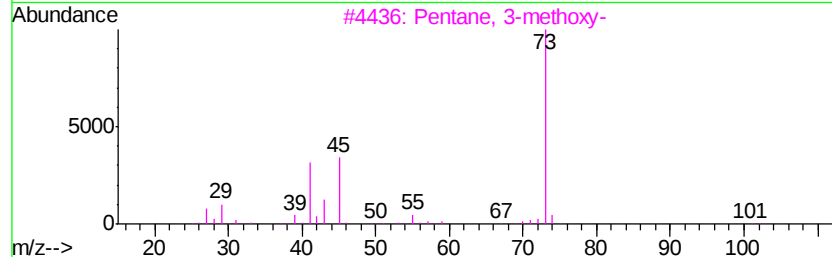
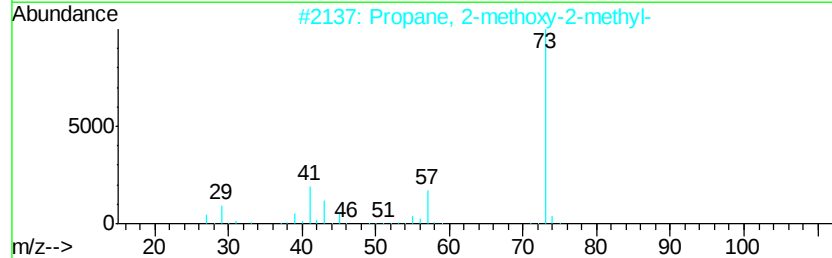
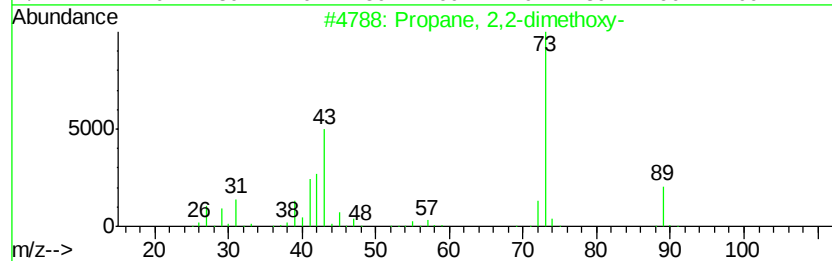
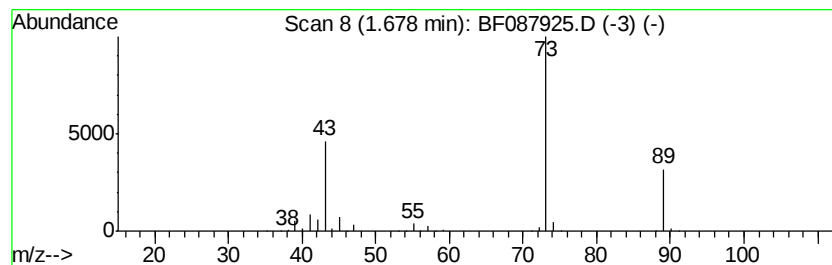
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	129.32 ng	3992820	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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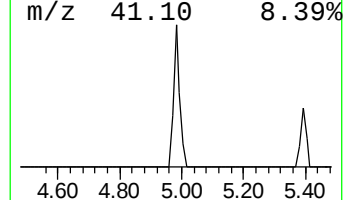
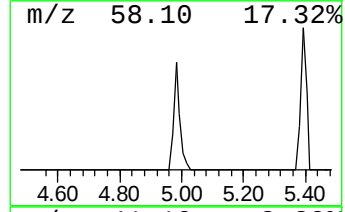
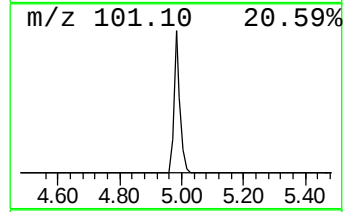
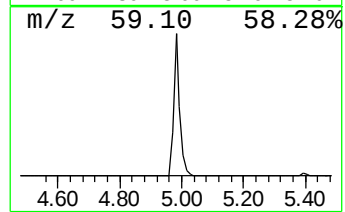
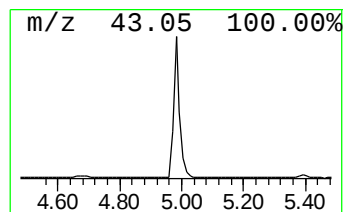
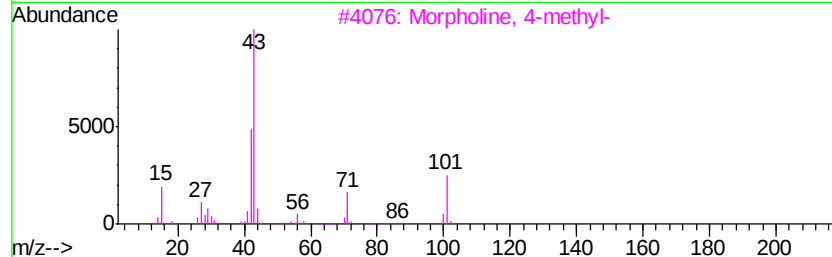
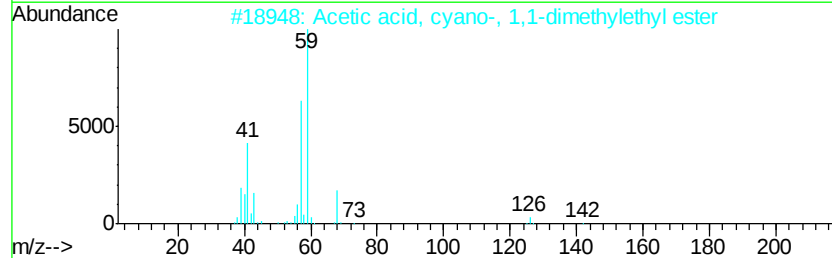
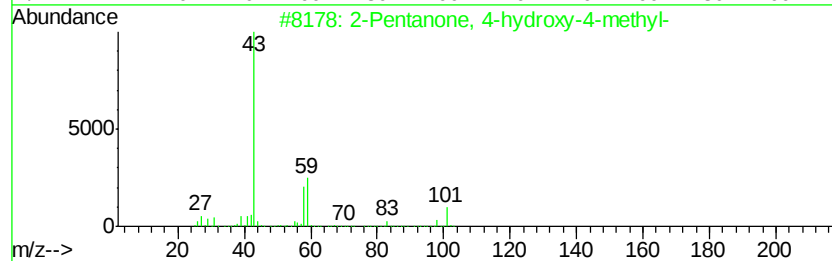
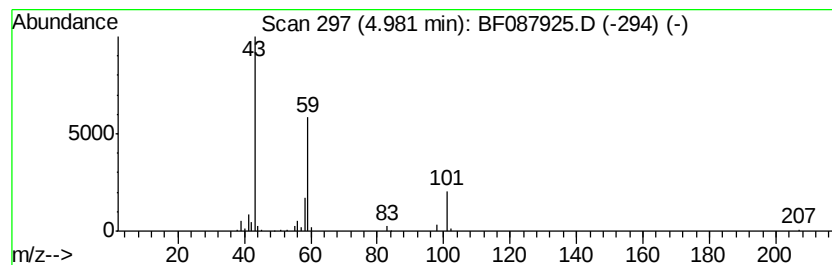
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	5.04 ng	155667	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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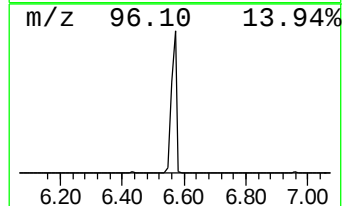
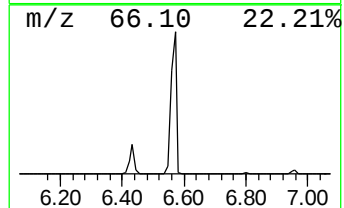
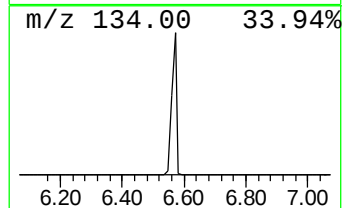
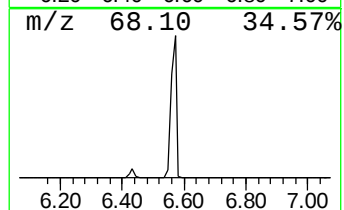
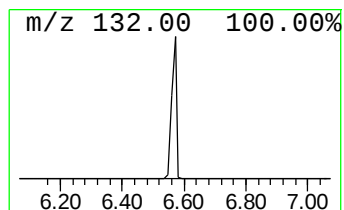
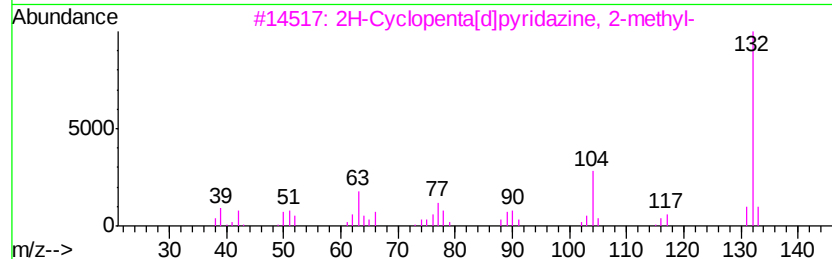
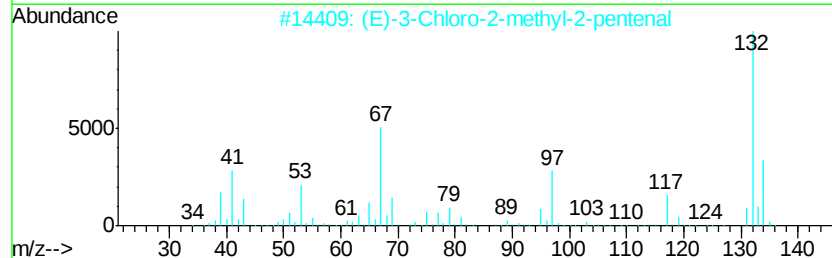
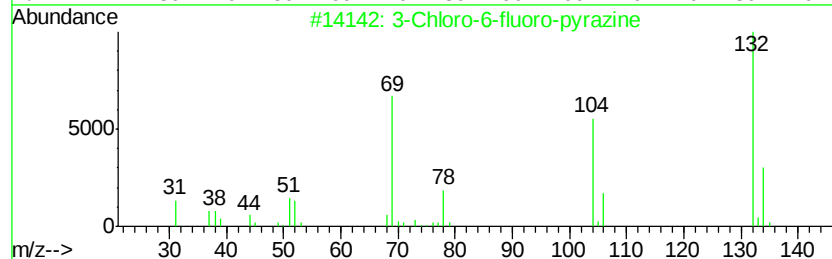
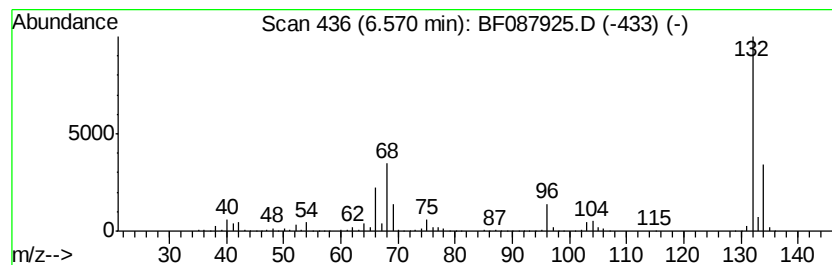
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Peak Number 5 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	83.08 ng	2565160	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	2H-Cyclopenta[d]		pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-6-fluoro		pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloro		pyrimidine	132	C4H2ClFN2	062802-42-0	9



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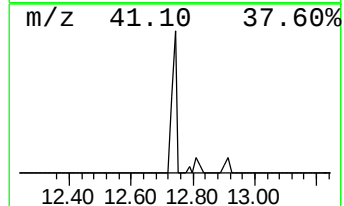
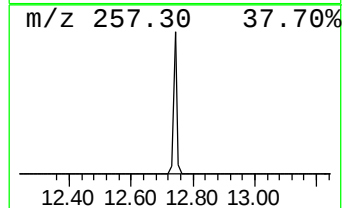
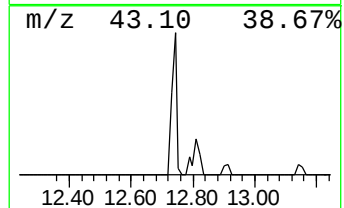
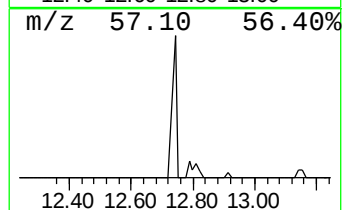
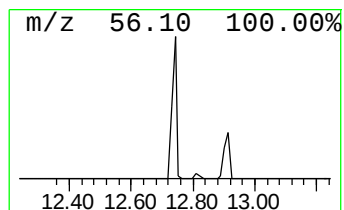
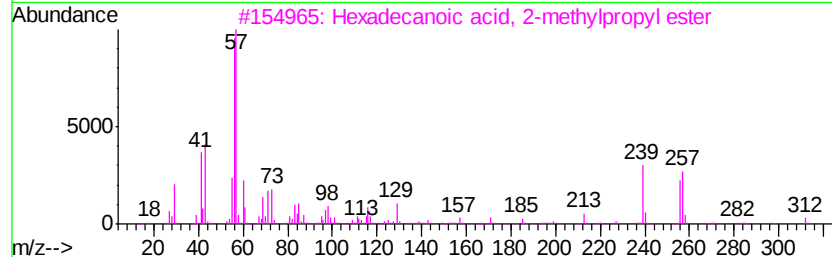
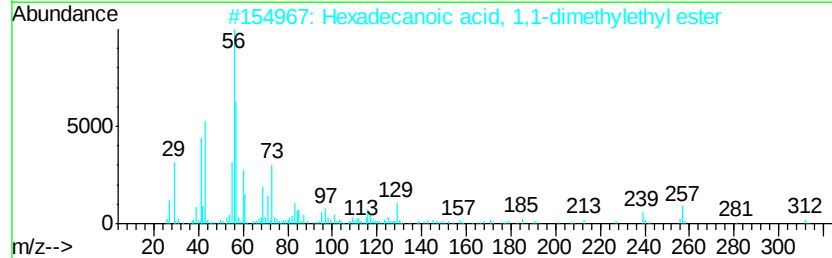
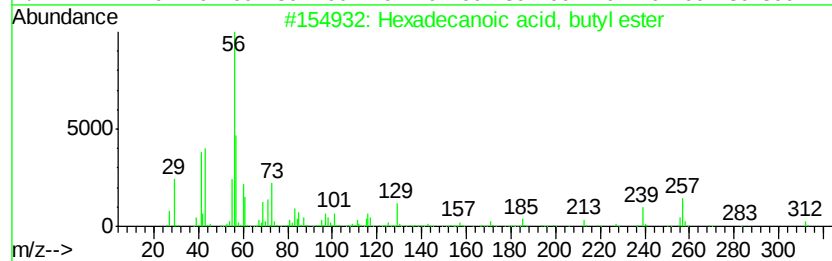
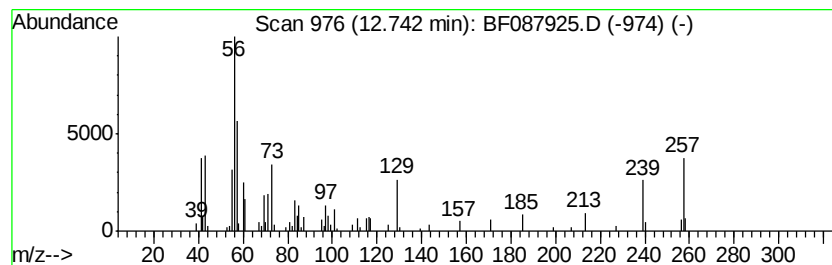
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.71 ng	128104	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	58
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.68	129.3	ng	3992820	1	6.80	617490	20.0
2-Pentanone, 4-hy...	4.98	5.0	ng	155667	1	6.80	617490	20.0
unknown6.57	6.57	83.1	ng	2565160	1	6.80	617490	20.0
Hexadecanoic acid...	12.74	2.7	ng	128104	5	13.95	946965	20.0