

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072916\
 Data File : BF089388.D
 Acq On : 29 Jul 2016 3:33
 Operator : UM/SJ
 Sample : H4221-12
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-46-6.0-7.0

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-BF072716.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	1.667	6	7	15	rVB	134873	258703	18.21%	1.890%
2	1.781	15	17	20	rBV	387340	599271	42.18%	4.378%
3	1.907	26	28	43	rVB	139130	219110	15.42%	1.601%
4	2.193	50	53	56	rVB	12073	19482	1.37%	0.142%
5	3.827	194	196	203	rBV	10431	24569	1.73%	0.179%
6	4.627	261	266	268	rBV	690325	1337426	94.13%	9.770%
7	5.096	304	307	309	rBV	957812	1281895	90.22%	9.364%
8	6.182	399	402	405	rBV	847008	1293398	91.03%	9.448%
9	6.296	409	412	414	rBV	1142007	1420808	100.00%	10.379%
10	6.525	430	432	443	rVB	233617	263617	18.55%	1.926%
11	6.673	443	445	448	rBV	797823	1018888	71.71%	7.443%
12	7.096	479	482	498	rBV	652647	830719	58.47%	6.068%
13	7.805	542	544	547	rBV	234251	336077	23.65%	2.455%
14	8.890	636	639	642	rBV	1442748	1410595	99.28%	10.304%
15	9.291	672	674	677	rBV	374025	320042	22.53%	2.338%
16	9.553	695	697	700	rBV	443037	389573	27.42%	2.846%
17	10.342	764	766	775	rBV	767066	759586	53.46%	5.549%
18	10.479	776	778	782	rVB	18109	19978	1.41%	0.146%
19	11.028	824	826	836	rVB	357087	340577	23.97%	2.488%
20	11.588	872	875	882	rBV2	11396	21815	1.54%	0.159%
21	12.605	962	964	967	rBV	676559	929247	65.40%	6.788%
22	13.520	1042	1044	1048	rBV2	25210	44442	3.13%	0.325%
23	13.645	1053	1055	1062	rVV	275796	279832	19.70%	2.044%
24	14.171	1098	1101	1104	rBV5	12718	17977	1.27%	0.131%
25	14.983	1170	1172	1179	rVB	202096	235661	16.59%	1.721%
26	16.960	1343	1345	1350	rVB3	6357	16167	1.14%	0.118%

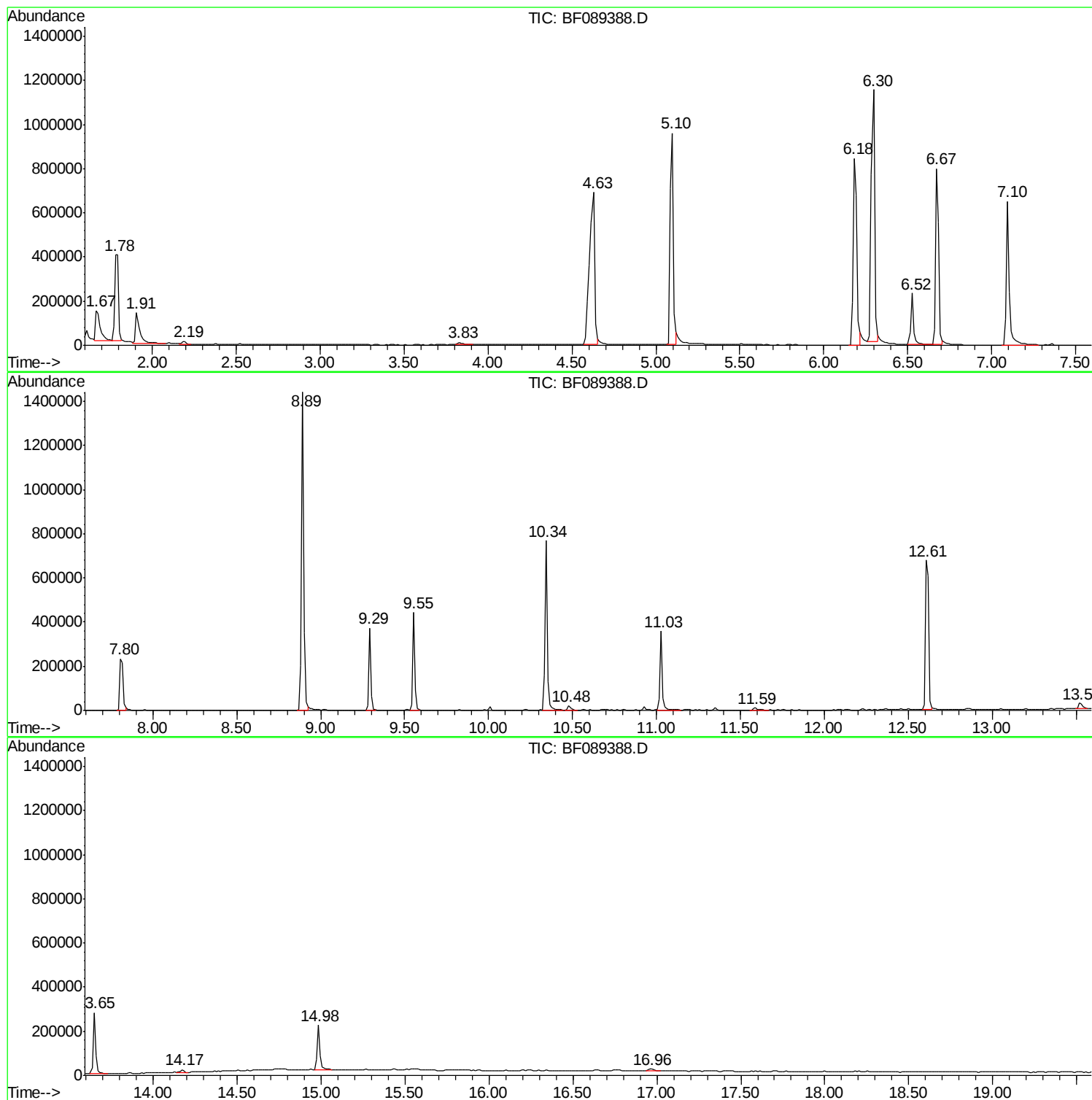
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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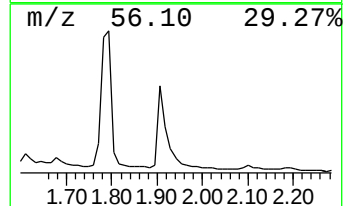
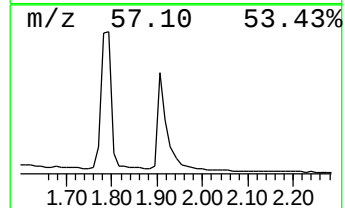
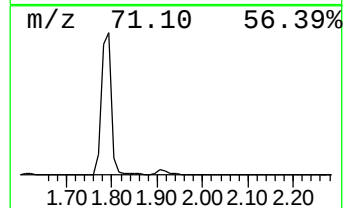
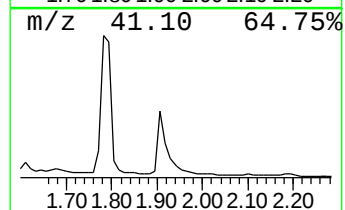
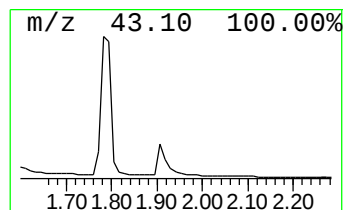
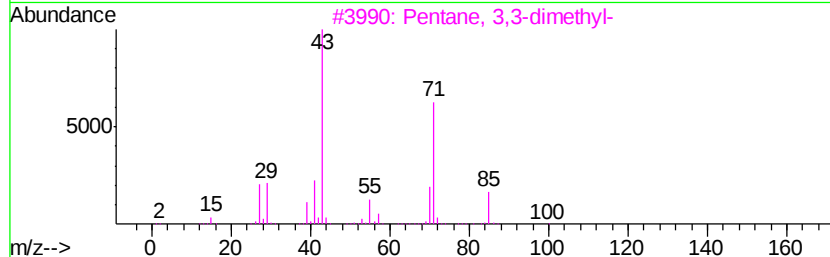
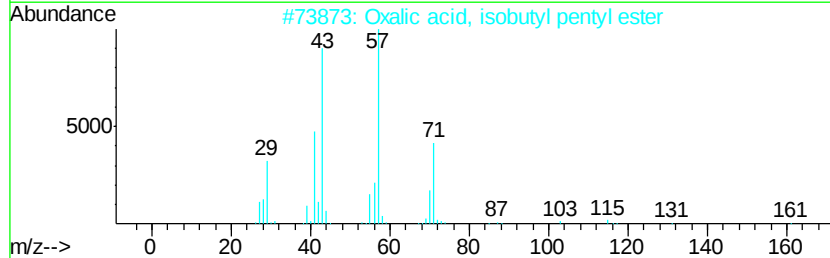
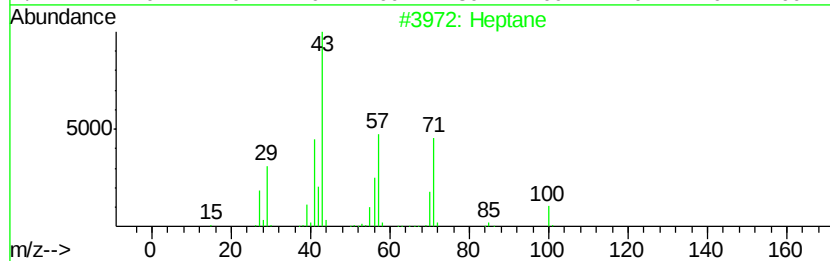
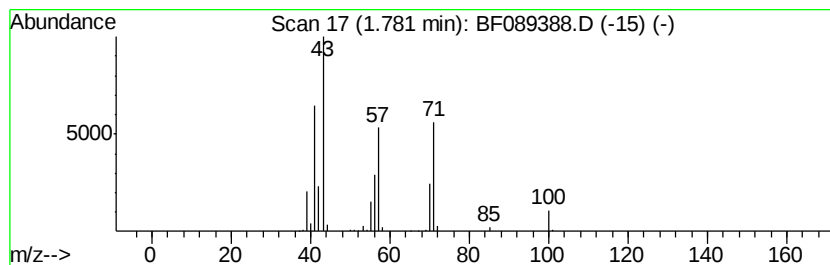
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	45.47 ng	599271	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	45
3		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38



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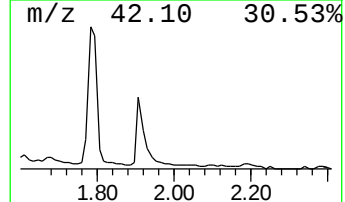
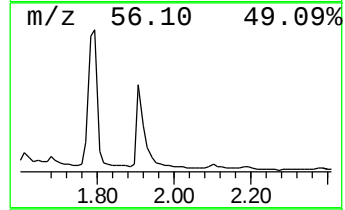
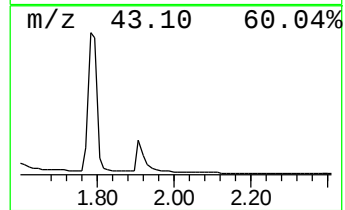
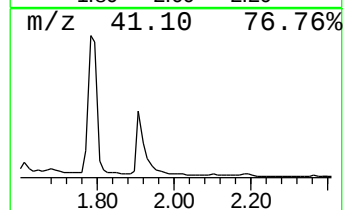
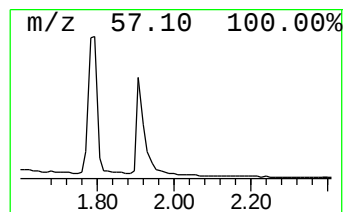
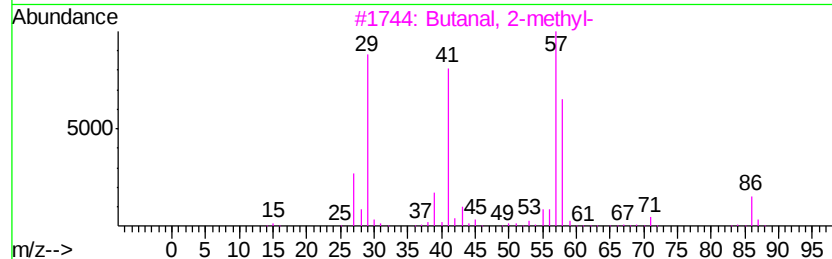
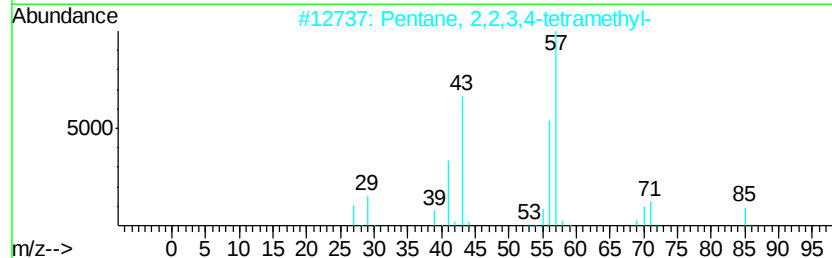
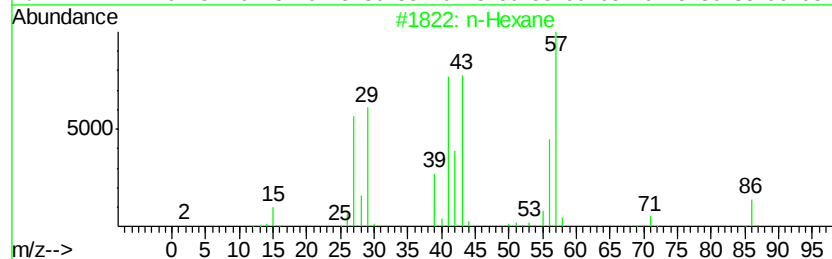
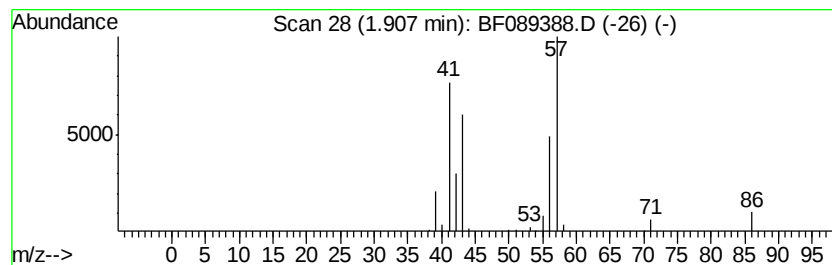
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Peak Number 3 n-Hexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	16.62 ng	219110	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	91
2		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
3		Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
4		Methane, isocyanato-	57	C2H3NO	000624-83-9	32
5		Pentane, 3-methyl-	86	C6H14	000096-14-0	28



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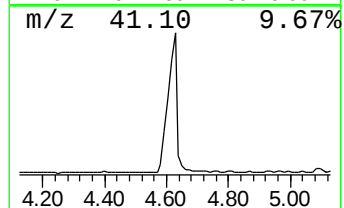
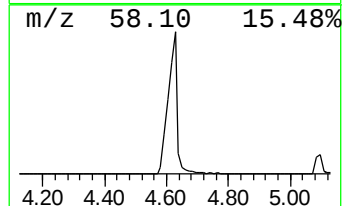
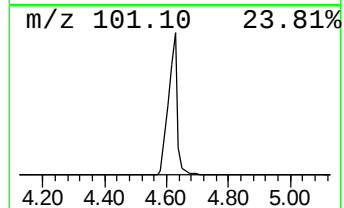
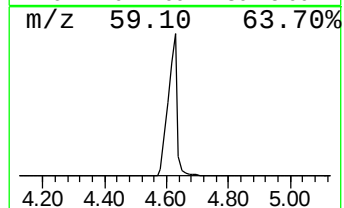
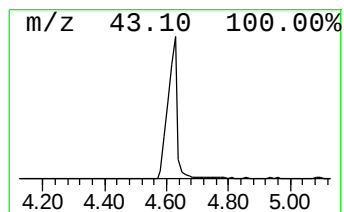
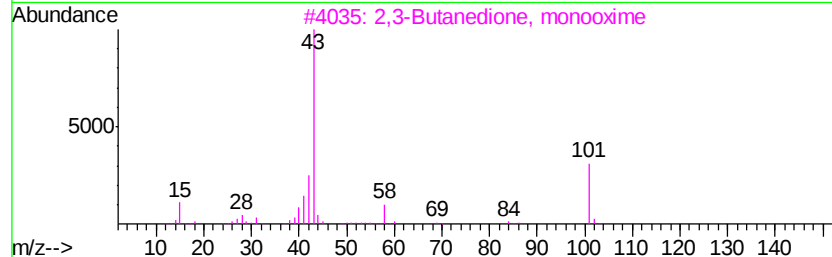
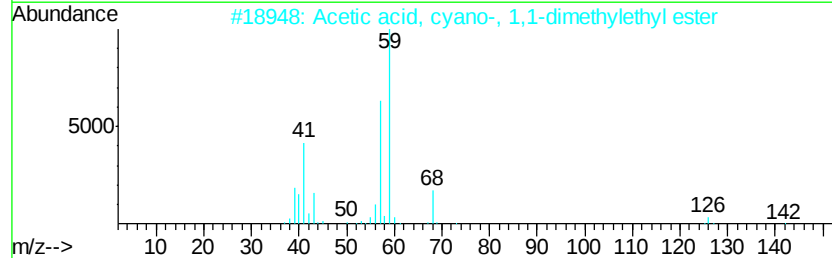
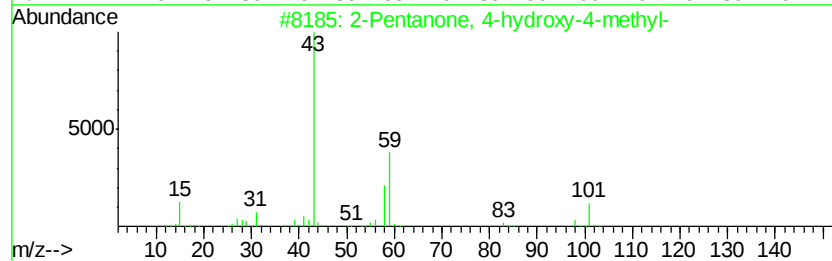
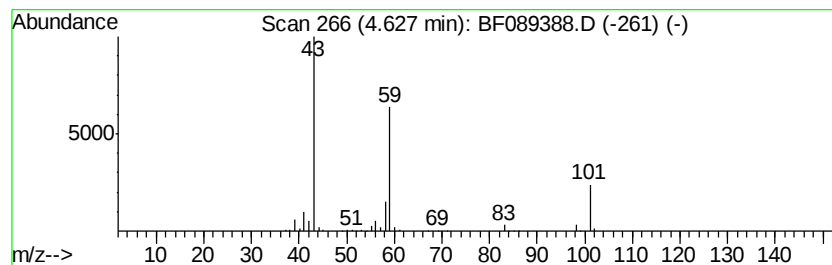
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	101.47 ng	1337430	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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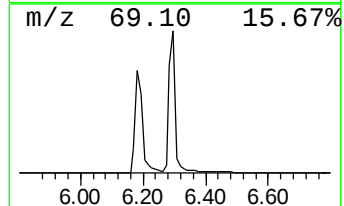
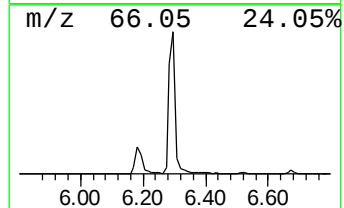
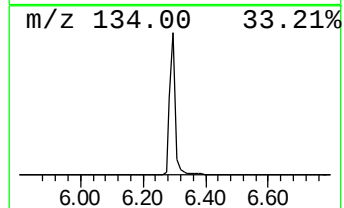
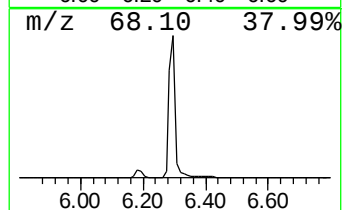
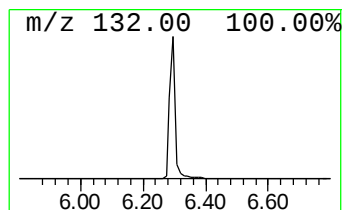
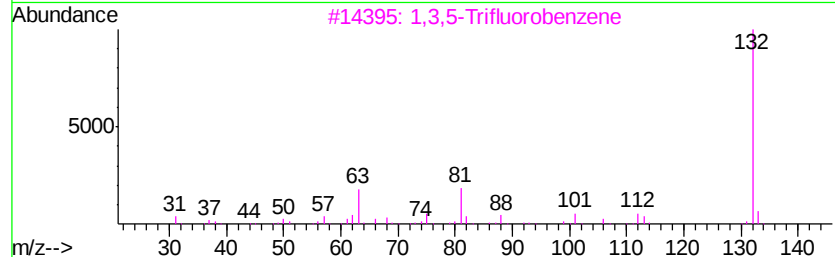
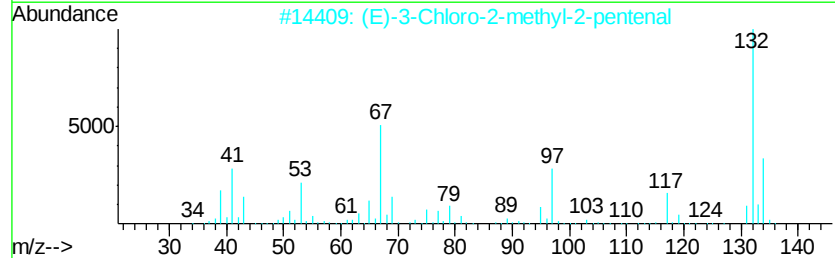
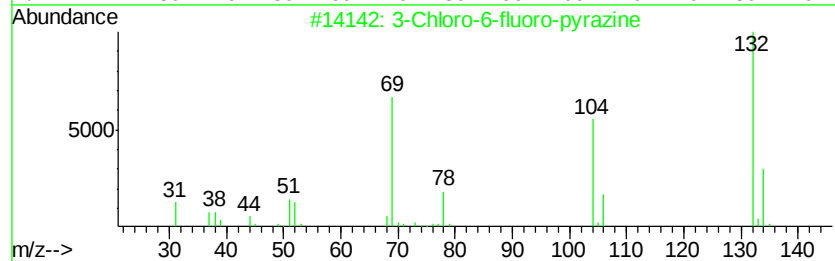
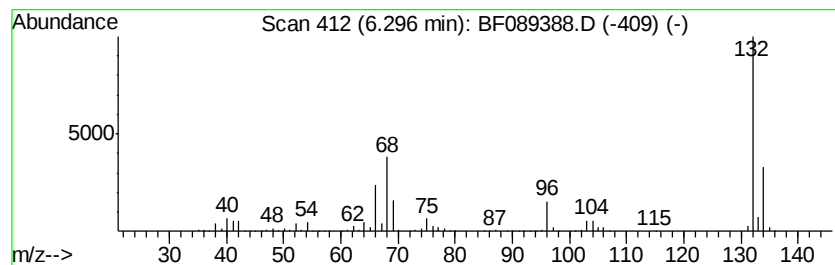
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Peak Number 5 unknown6.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	107.79 ng	1420810	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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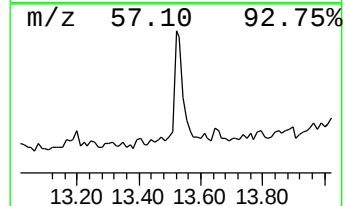
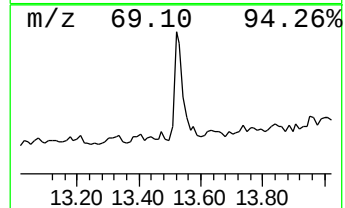
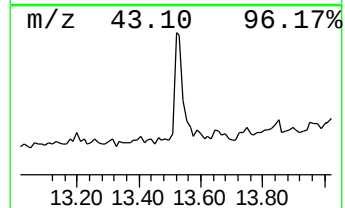
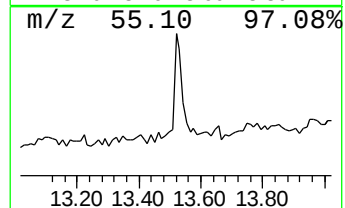
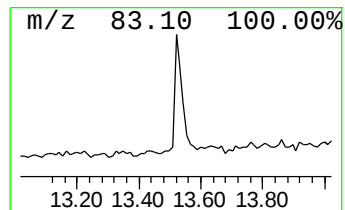
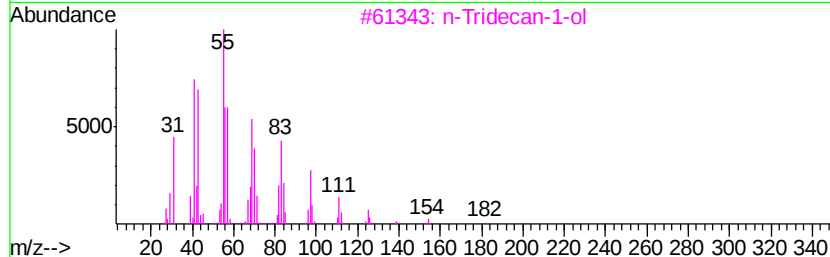
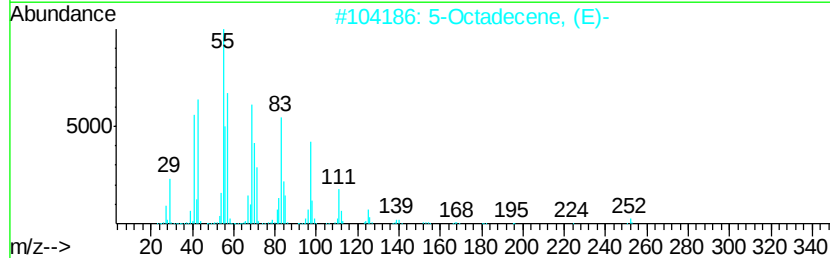
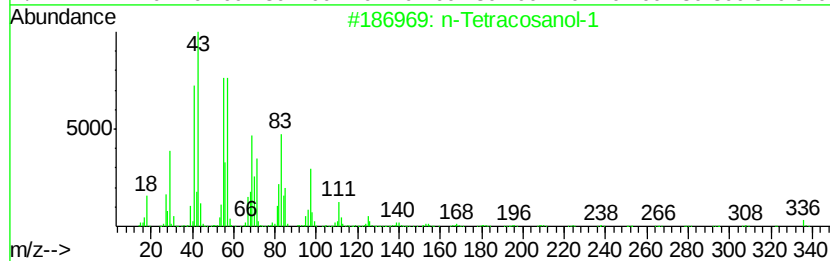
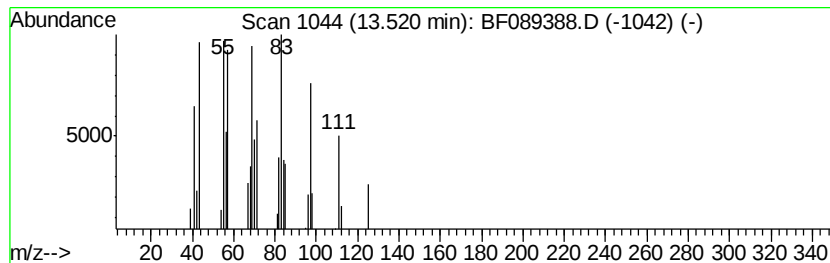
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Peak Number 7 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.52	3.18 ng	44442	Chrysene-d12	13.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	72
3	n-Tridecan-1-ol	200	C13H28O	000112-70-9	59
4	Cyclotetradecane	196	C14H28	000295-17-0	53
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptane	1.78	45.5	ng	599271	1	6.52	263617	20.0
n-Hexane	1.91	16.6	ng	219110	1	6.52	263617	20.0
2-Pentanone, 4-hy...	4.63	101.5	ng	1337430	1	6.52	263617	20.0
unknown6.30	6.30	107.8	ng	1420810	1	6.52	263617	20.0
n-Tetracosanol-1	13.52	3.2	ng	44442	5	13.65	279832	20.0