

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
 Data File : BF088947.D
 Acq On : 13 Jul 2016 6:20
 Operator : UM/SJ
 Sample : H3987-05
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-FLOOR-070816

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-BF063016.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	14	rVV	57415	86380	4.28%	0.554%
2	1.793	16	18	26	rVV	283731	392054	19.45%	2.513%
3	1.907	26	28	31	rVB	39672	46050	2.28%	0.295%
4	4.856	284	286	293	rBB	218354	361101	17.91%	2.314%
5	5.302	322	325	328	rBV	1413515	1632382	80.96%	10.463%
6	5.702	358	360	362	rBB	29336	24699	1.23%	0.158%
7	6.353	414	417	419	rBV	1461943	1638327	81.26%	10.501%
8	6.399	419	421	423	rVB	21555	21476	1.07%	0.138%
9	6.479	425	428	430	rBV	1636882	2004650	99.43%	12.849%
10	6.696	445	447	450	rBV	269514	360960	17.90%	2.314%
11	6.856	459	461	464	rVB	1237216	1293909	64.18%	8.293%
12	7.096	481	482	484	rBB	34400	28592	1.42%	0.183%
13	7.267	494	497	500	rBB	931791	1055856	52.37%	6.768%
14	7.987	557	560	562	rBV	590957	483610	23.99%	3.100%
15	9.073	652	655	657	rBV	1731118	2016206	100.00%	12.923%
16	9.462	687	689	691	rVB	402701	310033	15.38%	1.987%
17	9.736	711	713	715	rBB	533557	446490	22.15%	2.862%
18	10.525	779	782	784	rBV	947897	930497	46.15%	5.964%
19	10.651	792	793	798	rVB	17945	20838	1.03%	0.134%
20	10.971	819	821	824	rVB	24138	33134	1.64%	0.212%
21	11.211	840	842	844	rVB	437725	350330	17.38%	2.245%
22	12.799	978	981	983	rBV	1323431	1267495	62.87%	8.124%
23	13.279	1021	1023	1025	rBV	37133	53072	2.63%	0.340%
24	13.702	1057	1060	1063	rBV	48393	55468	2.75%	0.356%
25	13.839	1069	1072	1074	rBV	303739	353244	17.52%	2.264%
26	13.965	1078	1083	1086	rBV	10023	21102	1.05%	0.135%
27	14.331	1113	1115	1121	rBV2	19173	29827	1.48%	0.191%
28	15.211	1189	1192	1194	rBV	211217	284003	14.09%	1.820%

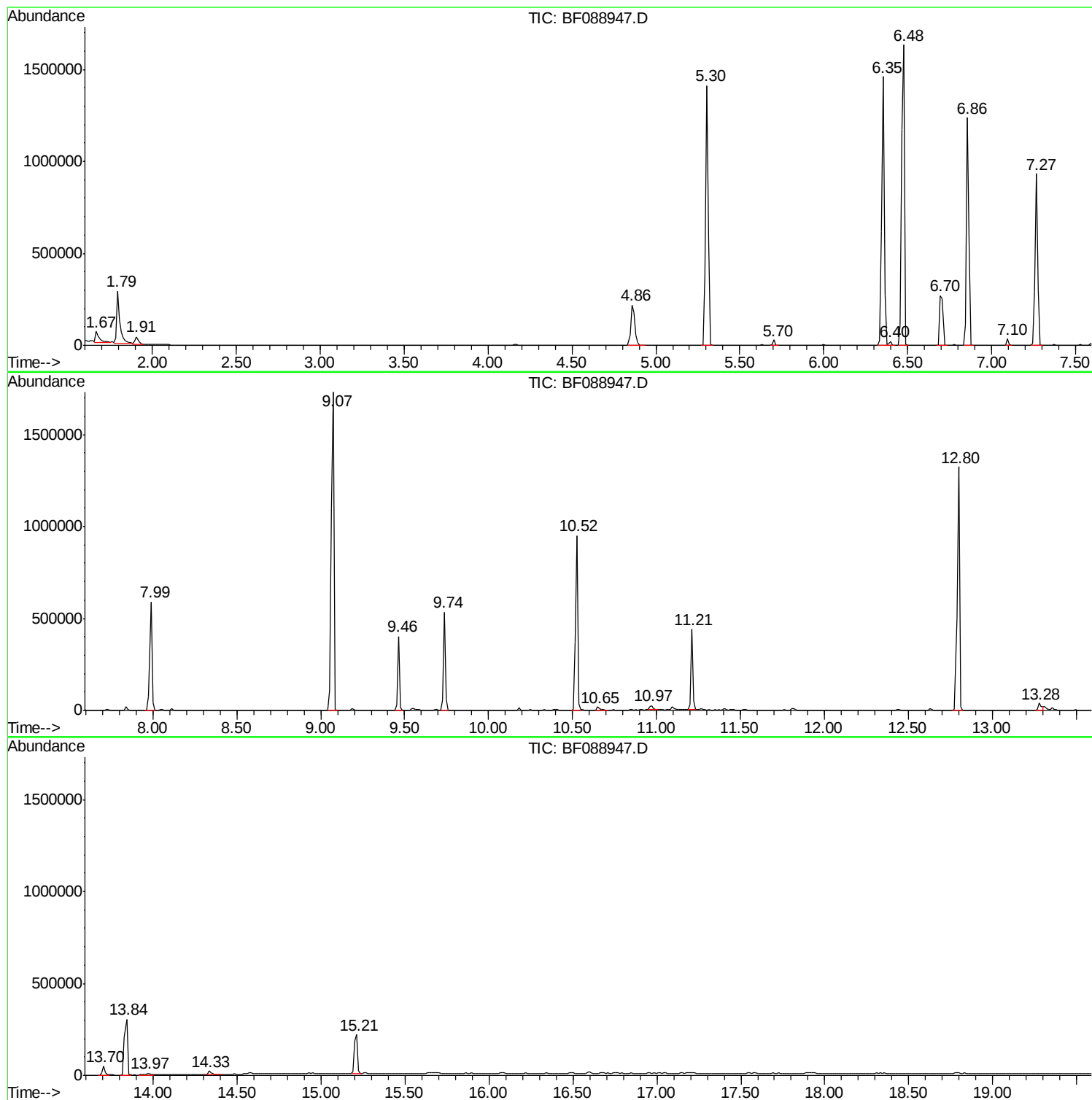
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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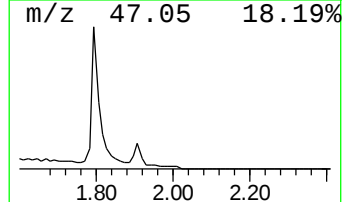
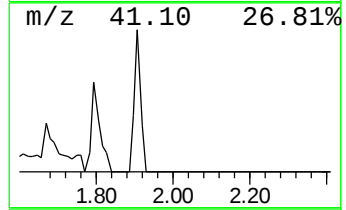
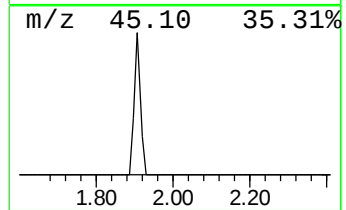
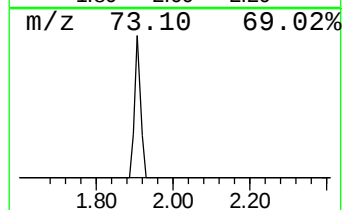
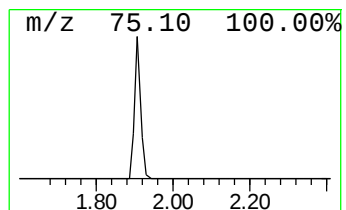
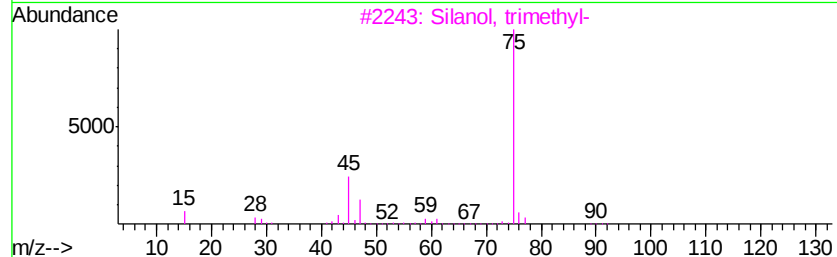
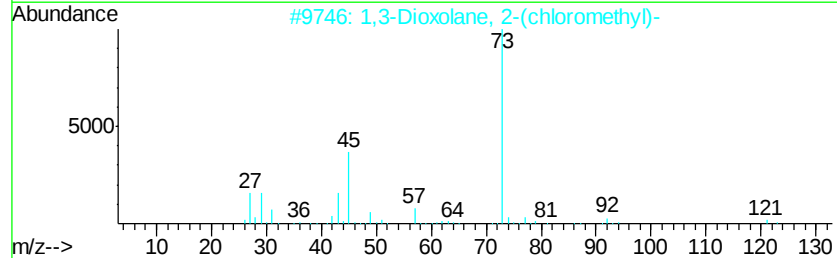
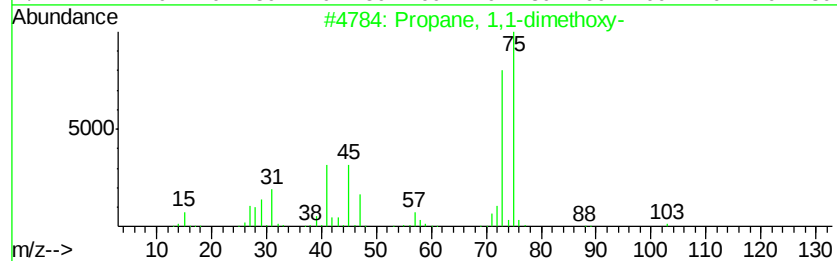
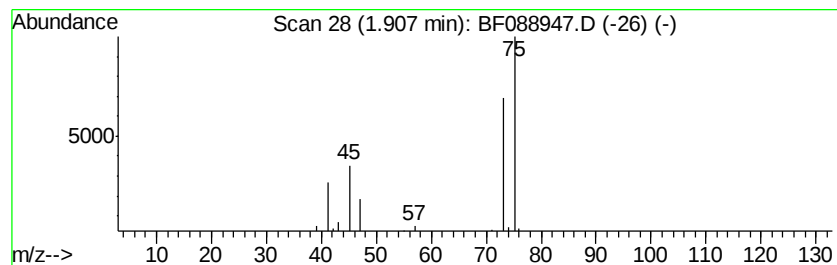
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	2.55 ng	46050	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9



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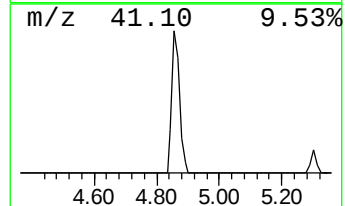
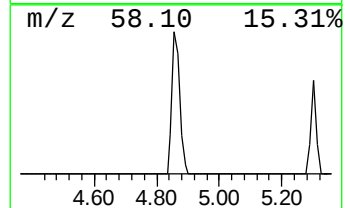
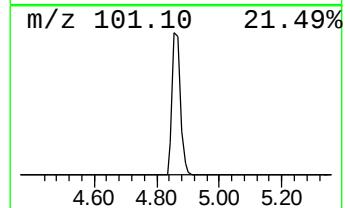
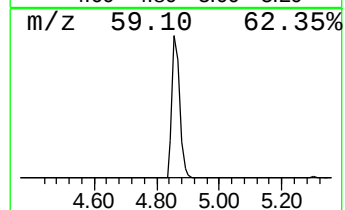
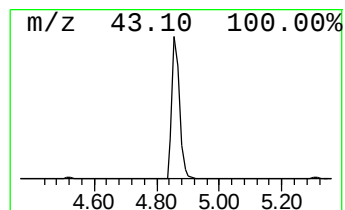
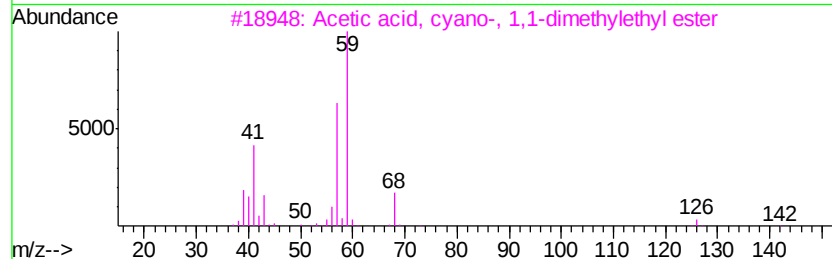
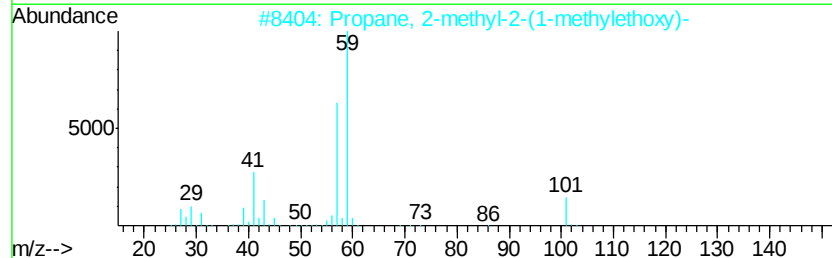
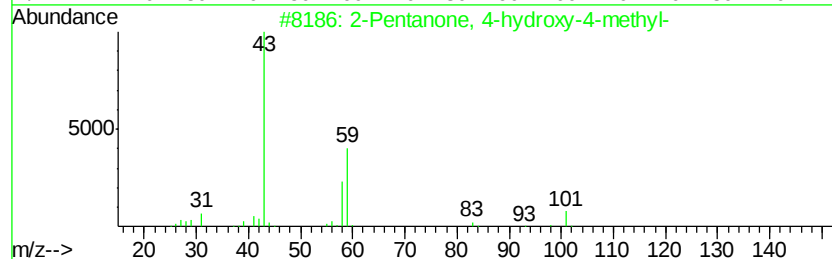
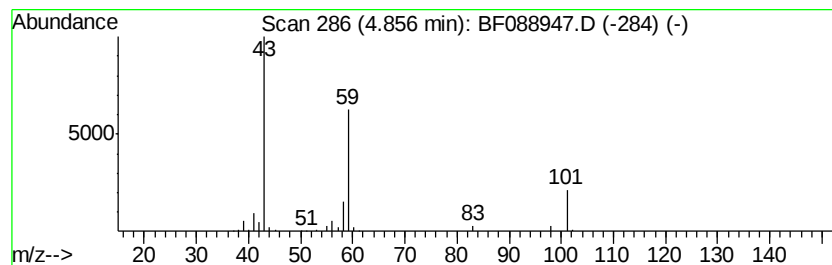
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	20.01 ng	361101	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		(+)-4-Amino-4,5-dihydro-2(3H)-furan	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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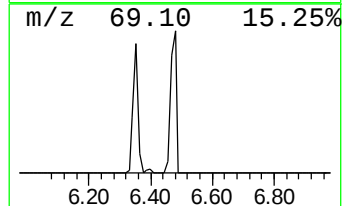
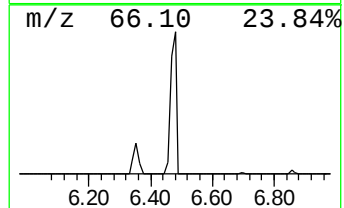
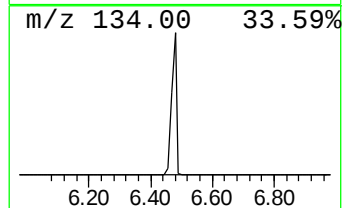
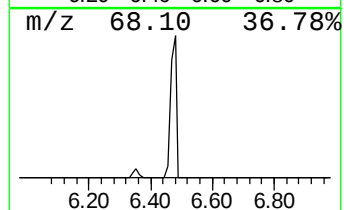
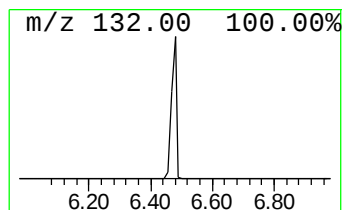
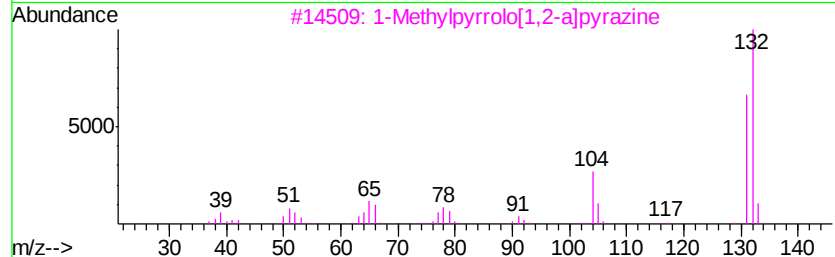
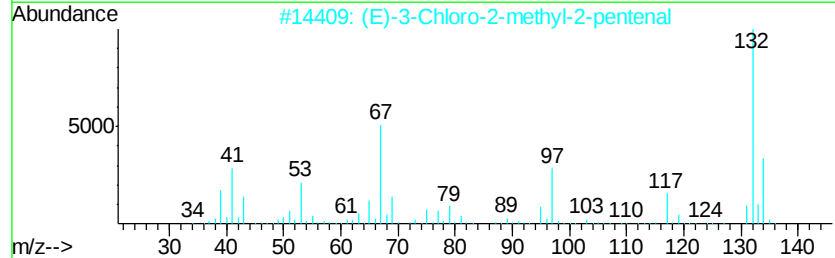
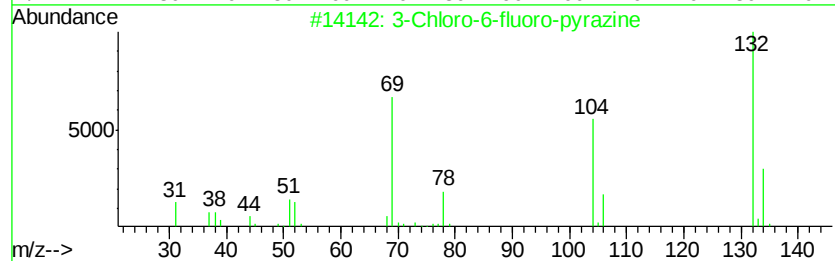
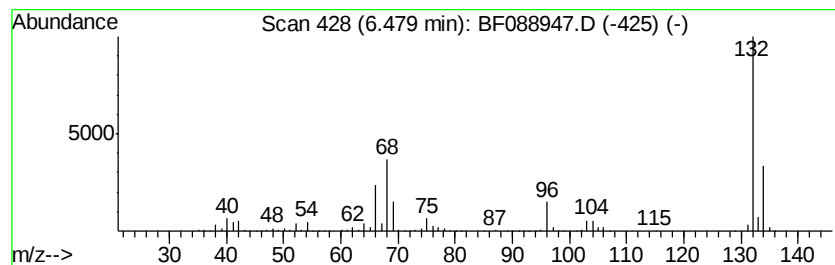
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	111.07 ng	2004650	1,4-Dichlorobenzene-d4	6.71

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	25
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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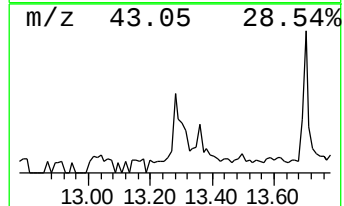
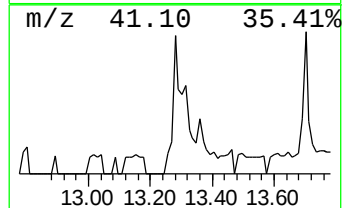
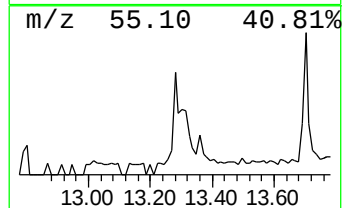
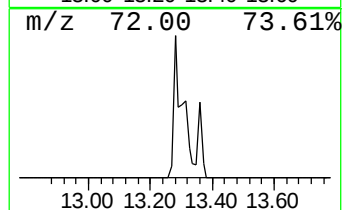
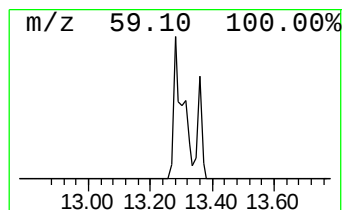
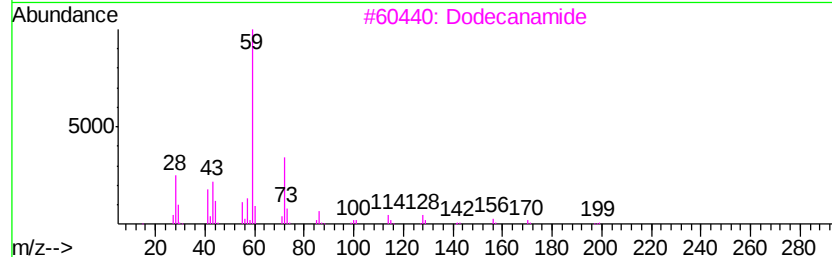
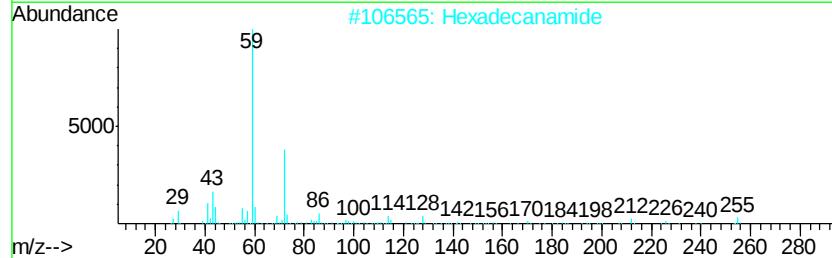
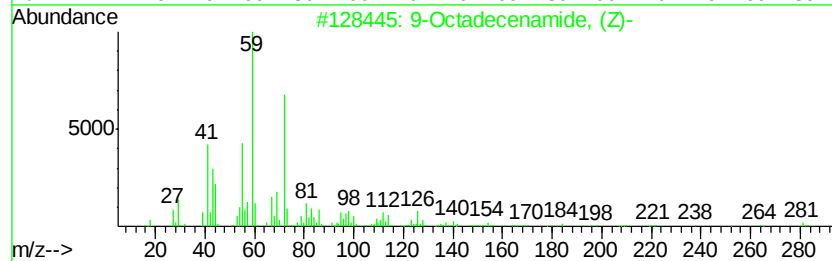
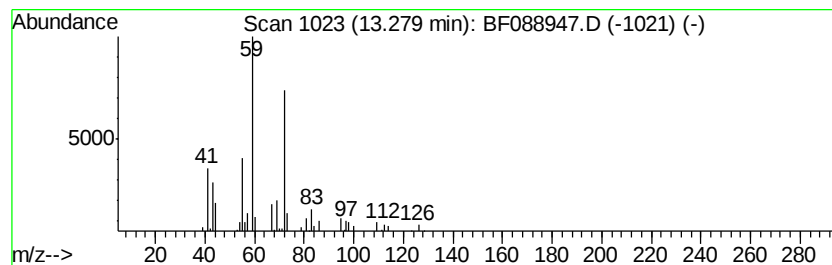
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	3.00 ng	53072	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	50
3		Dodecanamide	199	C12H25NO	001120-16-7	43
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	38
5		Silane, octyl-	144	C8H20Si	000871-92-1	32



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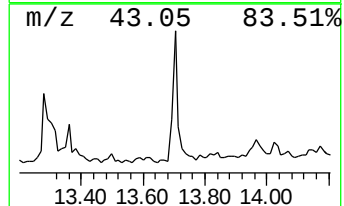
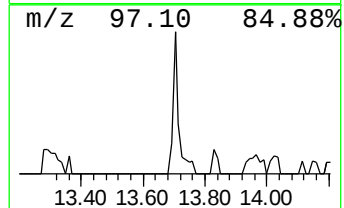
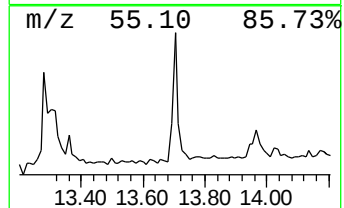
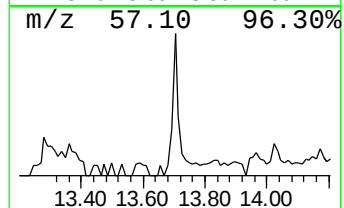
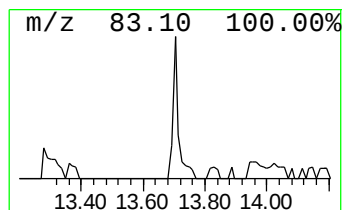
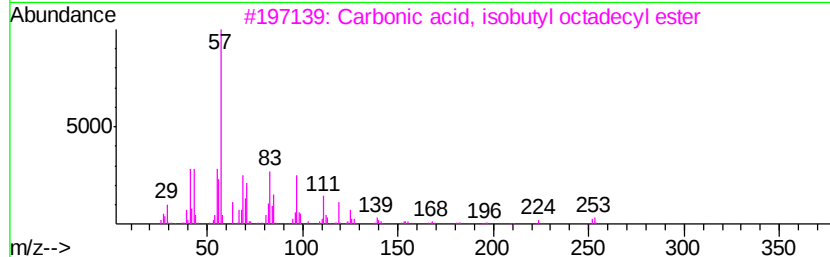
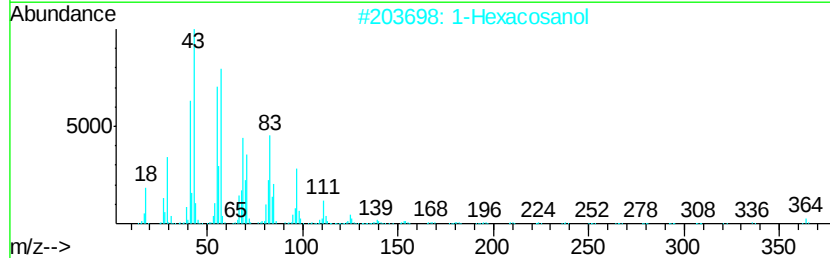
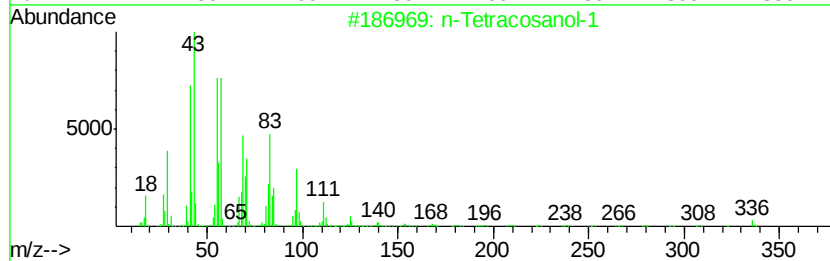
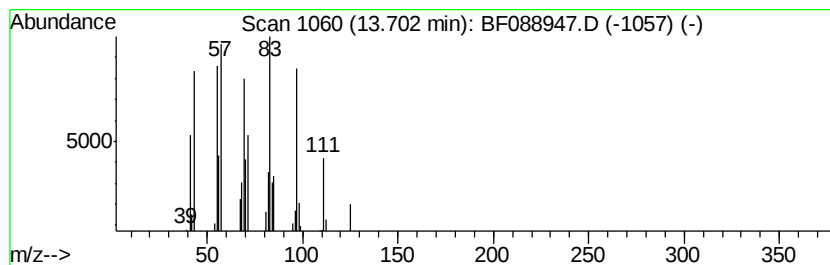
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Peak Number 8 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.70	3.14 ng	55468	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2	1-Hexacosanol	382	C26H54O	000506-52-5	74
3	Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	64
4	Cyclotetradecane	196	C14H28	000295-17-0	58
5	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.91	2.5	ng	46050	1	6.71	360960	20.0
2-Pentanone, 4-hy...	4.86	20.0	ng	361101	1	6.71	360960	20.0
unknown6.48	6.48	111.1	ng	2004650	1	6.71	360960	20.0
9-Octadecenamide, ...	13.28	3.0	ng	53072	5	13.84	353244	20.0
n-Tetracosanol-1	13.70	3.1	ng	55468	5	13.84	353244	20.0