

Data Path : Z:\HPCHEM1\BNA F\Data\BF112217\
 Data File : BF100840.D
 Acq On : 22 Nov 2017 23:01
 Operator : SJ/JU
 Sample : I6513-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :

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	3.846	291	299	318	rBV	1065712	1666299	100.00%	28.322%
2	5.046	500	503	508	rBV	24677	24937	1.50%	0.424%
3	5.463	570	574	586	rBV	383107	372371	22.35%	6.329%
4	6.481	744	747	755	rBV	450311	388001	23.29%	6.595%
5	6.622	768	771	775	rBV	464409	395287	23.72%	6.719%
6	6.857	808	811	815	rBV	98777	79950	4.80%	1.359%
7	7.010	834	837	841	rBV	384675	298092	17.89%	5.067%
8	7.416	902	906	909	rBV	322221	230800	13.85%	3.923%
9	8.139	1026	1029	1032	rBV	141183	102942	6.18%	1.750%
10	9.210	1208	1211	1215	rBV	556859	462786	27.77%	7.866%
11	9.604	1275	1278	1281	rBV	43747	32782	1.97%	0.557%
12	9.816	1309	1314	1319	rVB	19606	21193	1.27%	0.360%
13	9.892	1324	1327	1331	rVB	153423	128316	7.70%	2.181%
14	10.310	1394	1398	1403	rVB2	24398	32463	1.95%	0.552%
15	10.680	1458	1461	1465	rVB	398569	306495	18.39%	5.209%
16	11.380	1577	1580	1583	rBV	164607	131498	7.89%	2.235%
17	11.898	1664	1668	1673	rBV	89561	82079	4.93%	1.395%
18	12.680	1798	1801	1808	rBV	46970	47932	2.88%	0.815%
19	12.963	1845	1849	1852	rBV	667455	521662	31.31%	8.867%
20	13.851	1996	2000	2003	rBV2	51495	51970	3.12%	0.883%
21	13.886	2003	2006	2010	rVB	21690	20041	1.20%	0.341%
22	13.992	2020	2024	2026	rBV	297503	236728	14.21%	4.024%
23	14.021	2026	2029	2032	rVB	145944	131761	7.91%	2.240%
24	15.486	2275	2278	2285	rVB	89251	117036	7.02%	1.989%

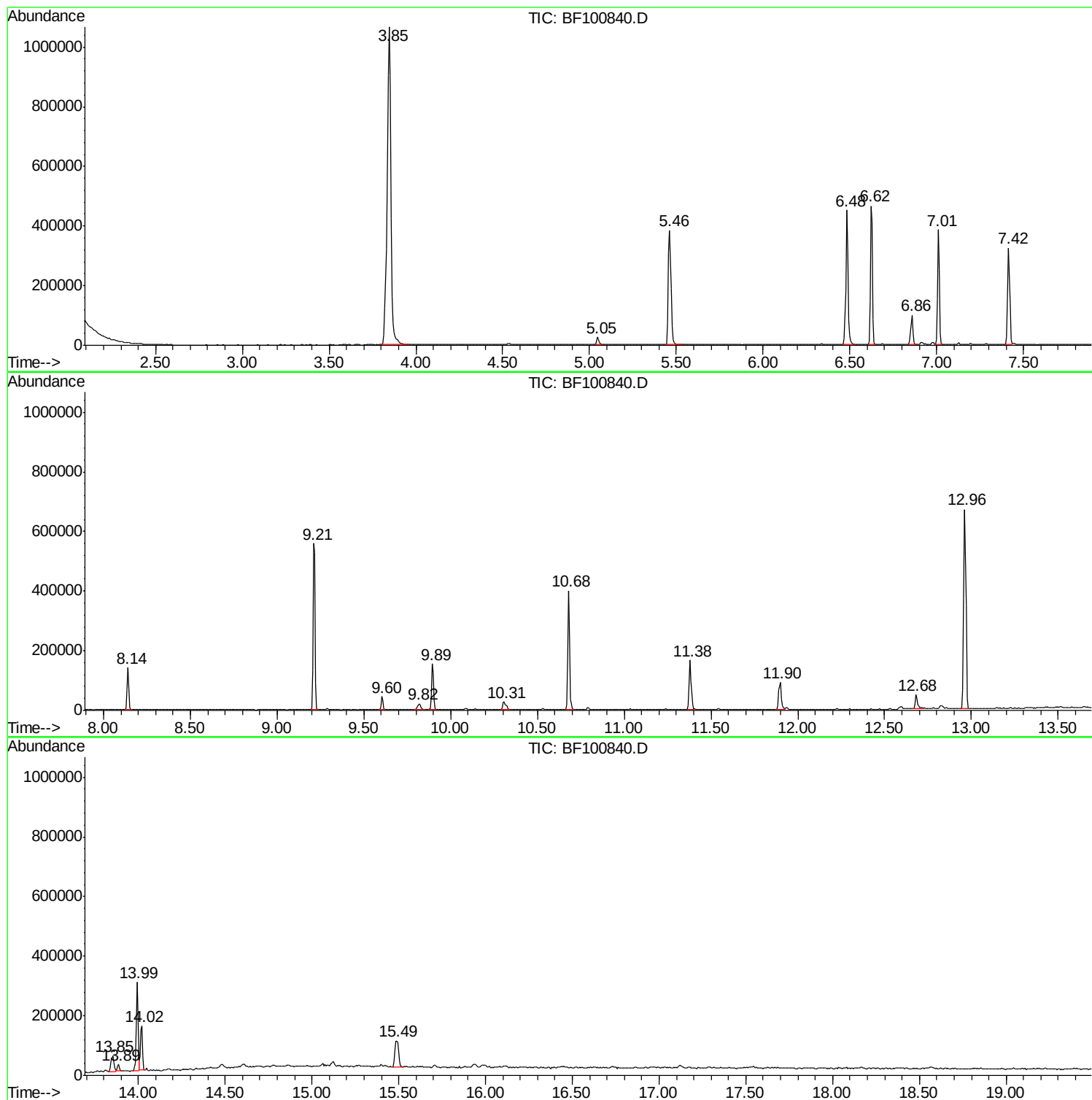
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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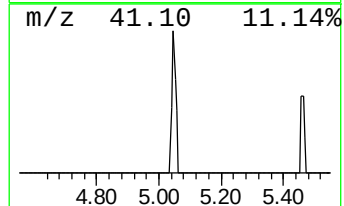
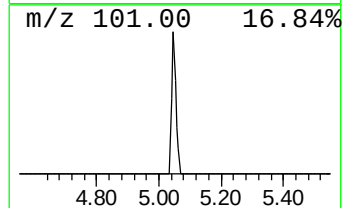
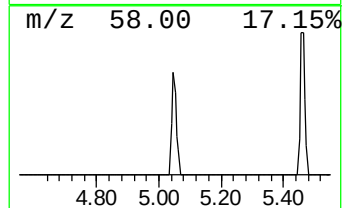
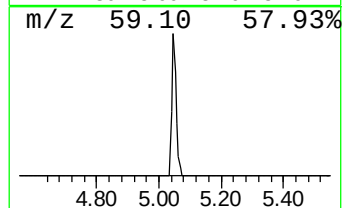
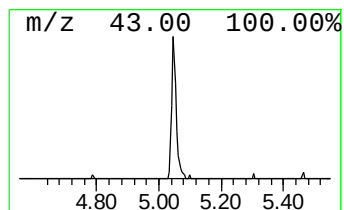
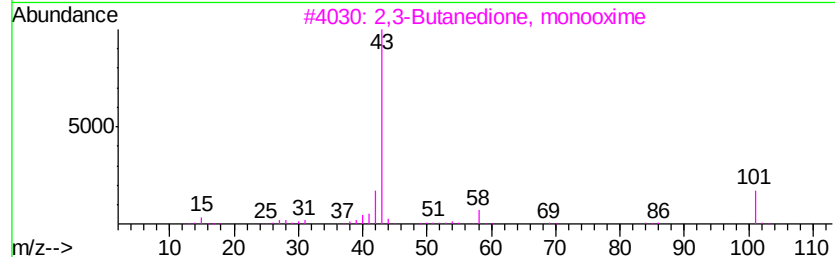
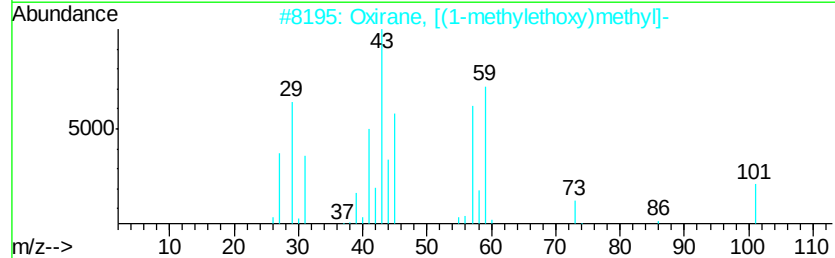
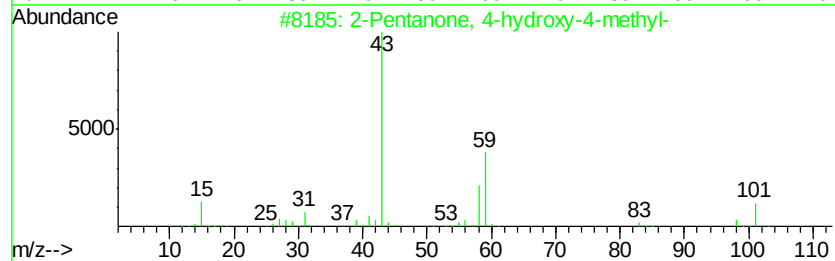
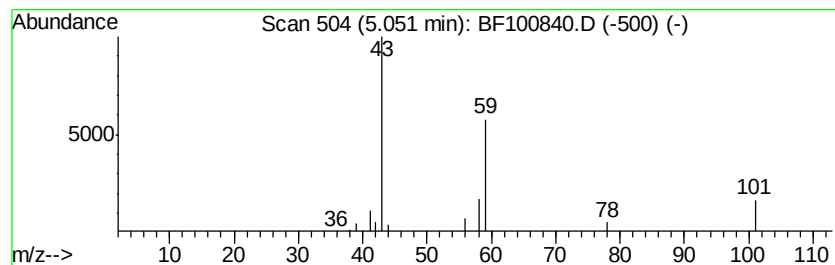
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.05	6.24 ng	24937	1,4-Dichlorobenzene-d4	6.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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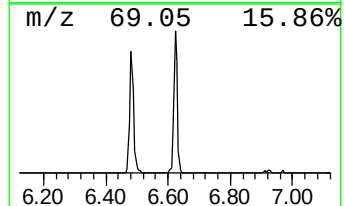
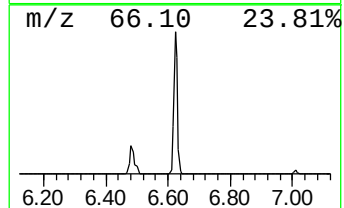
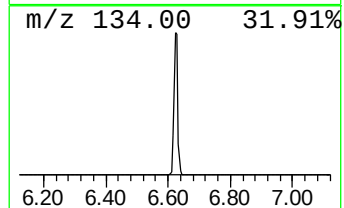
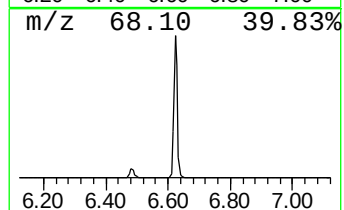
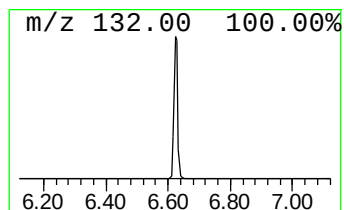
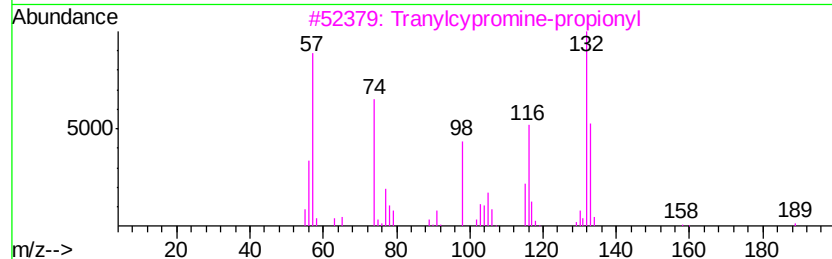
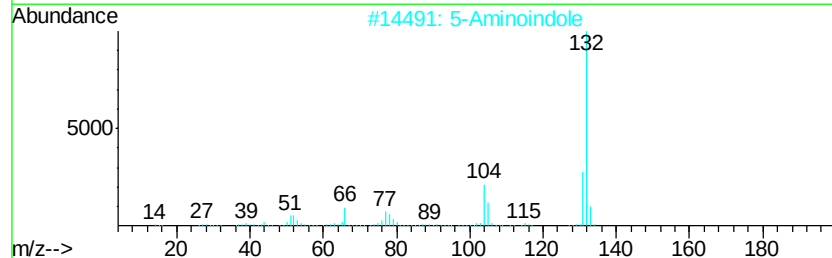
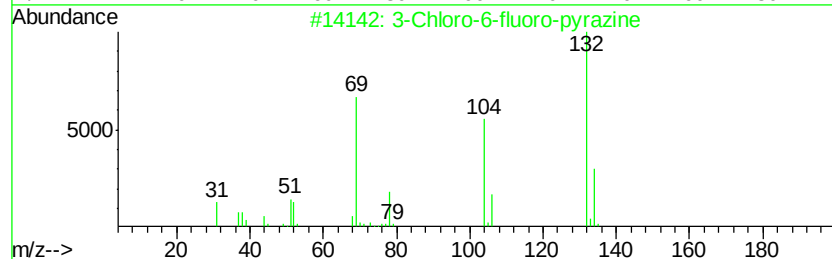
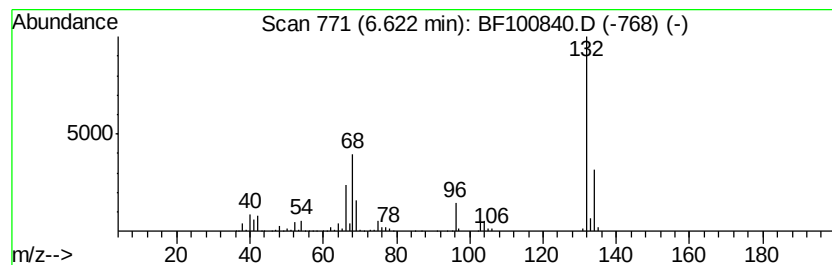
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Peak Number 3 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	98.88 ng	395287	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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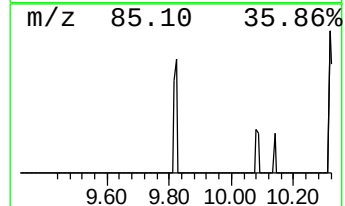
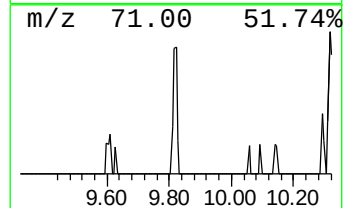
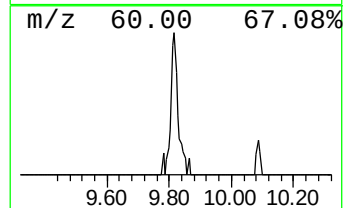
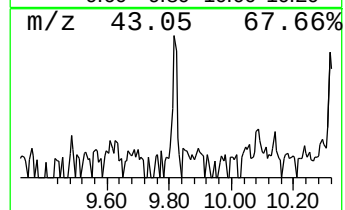
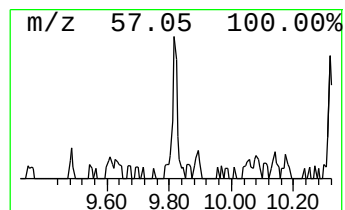
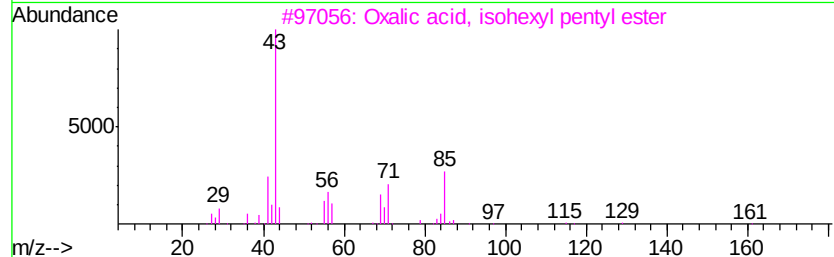
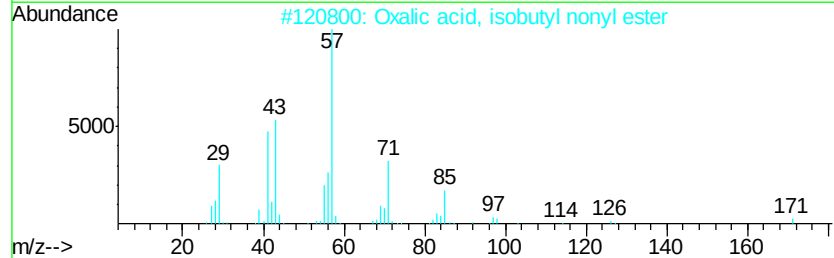
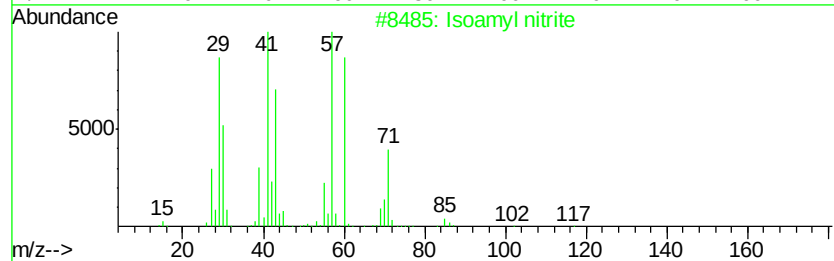
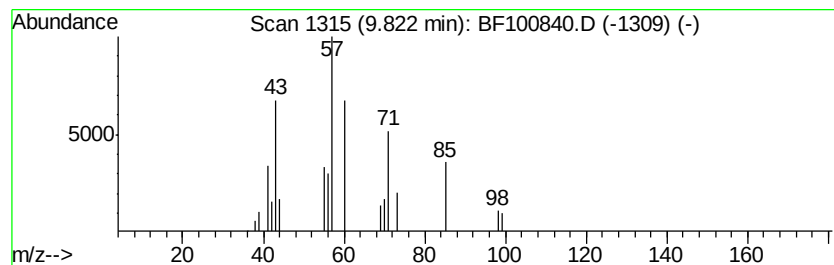
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Peak Number 5 unknown9.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	3.30 ng	21193	Acenaphthene-d10	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoamyl nitrite	117	C5H11NO2	000110-46-3	36
2		Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	32
3		Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	27
4		Acetamide, N-(2-hydroxyethyl)-	103	C4H9NO2	000142-26-7	23
5		.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	17



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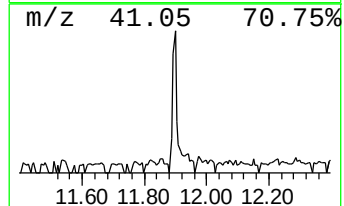
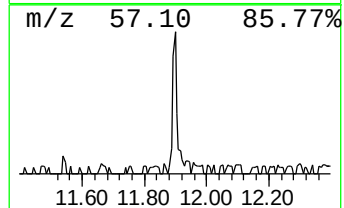
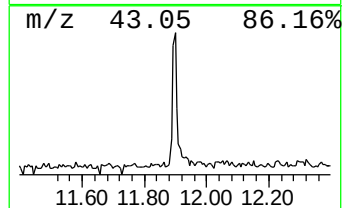
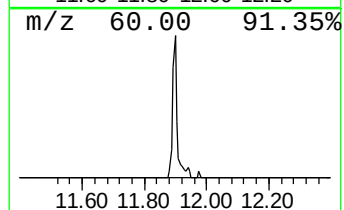
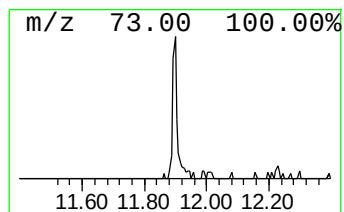
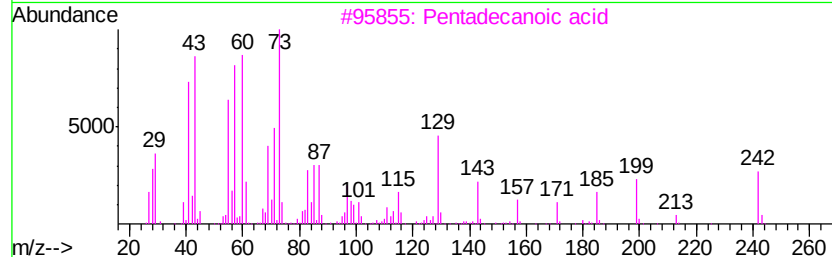
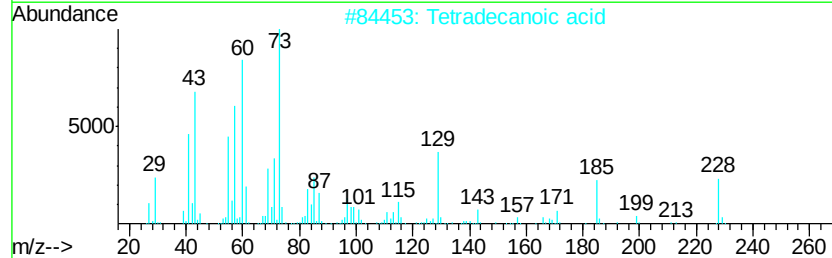
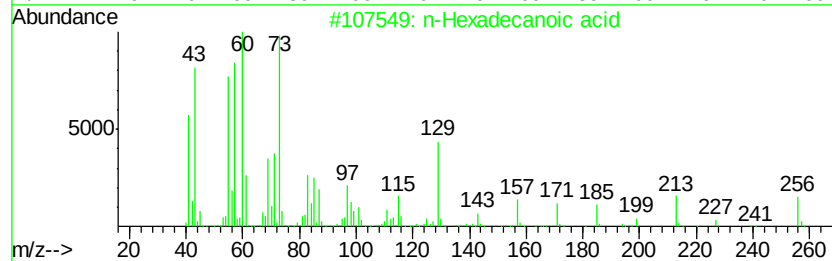
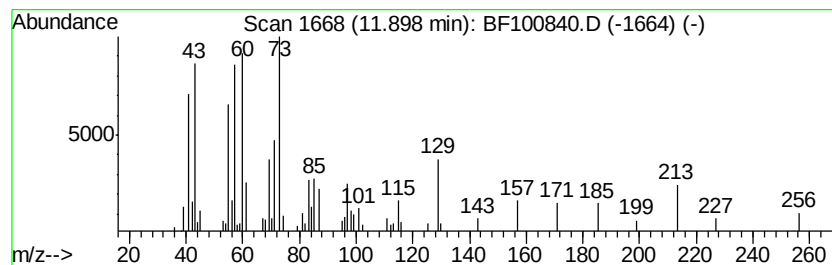
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	12.48 ng	82079	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



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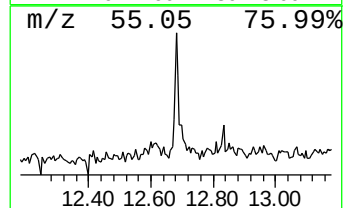
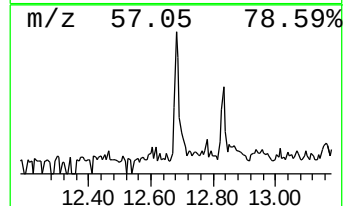
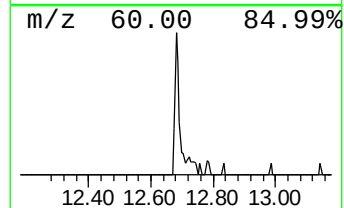
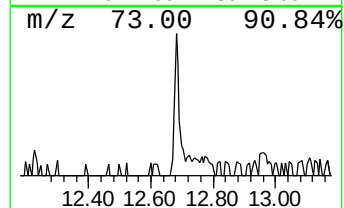
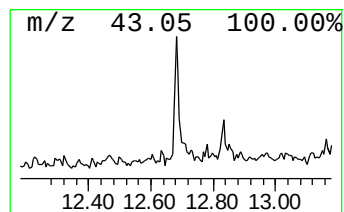
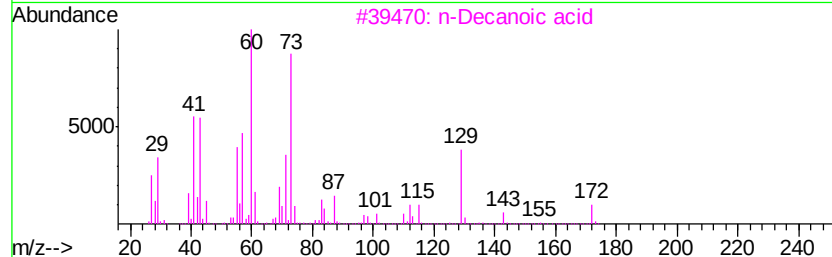
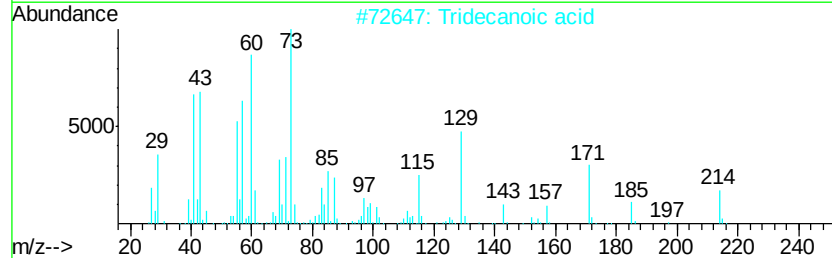
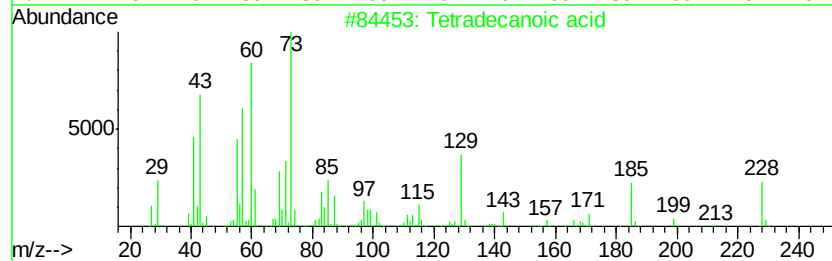
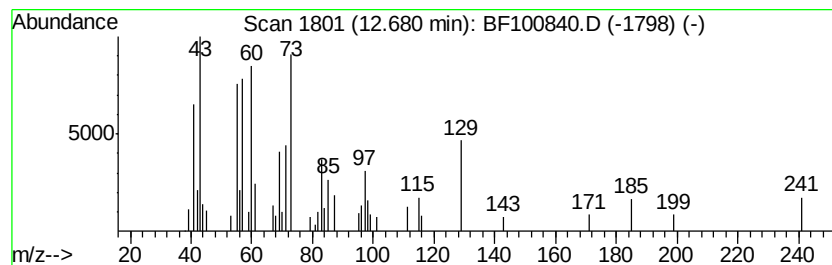
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Peak Number 7 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	7.29 ng	47932	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	35
5		Xylose	150	C5H10O5	000058-86-6	27



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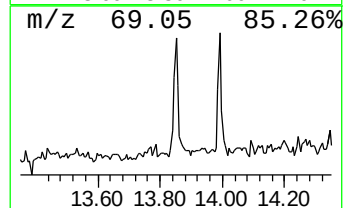
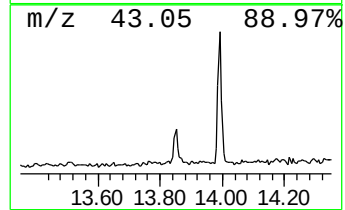
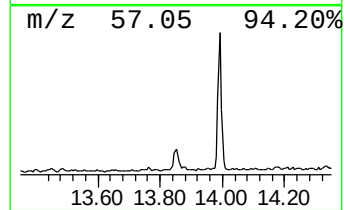
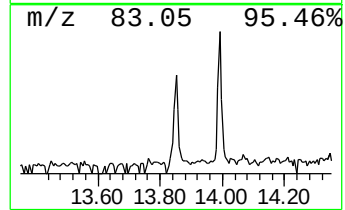
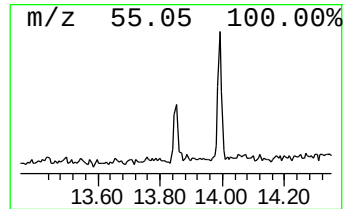
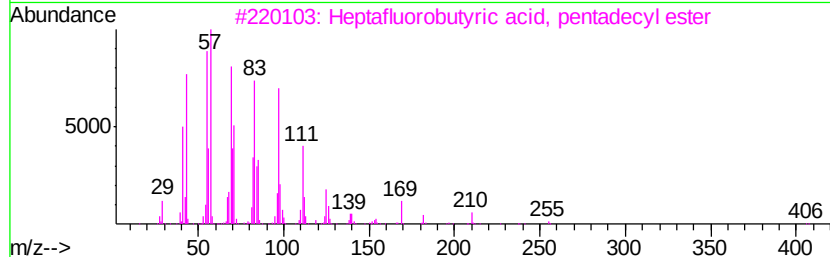
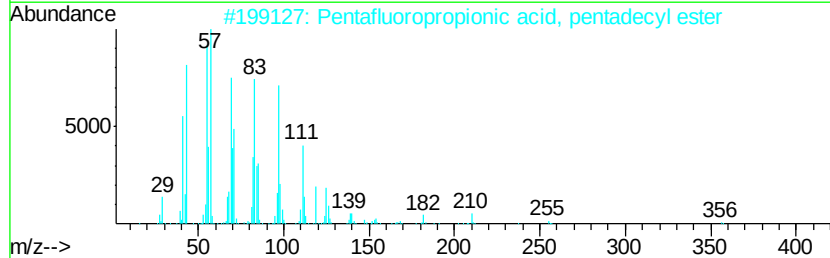
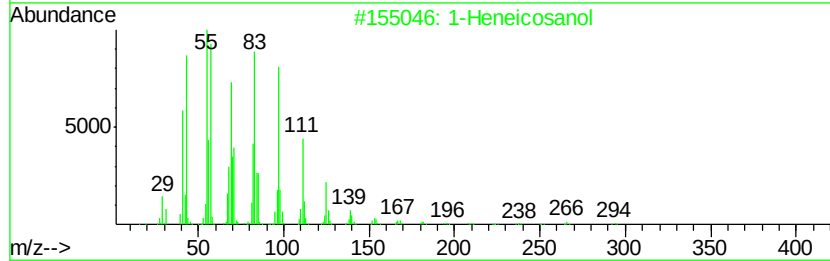
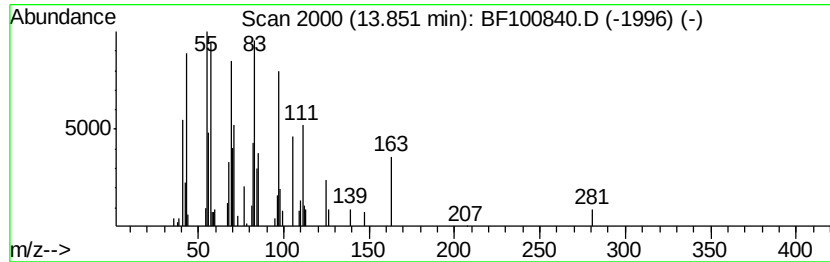
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	7.89 ng	51970	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90



Data Path : Z:\HPCHEM1\BNA F\Data\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

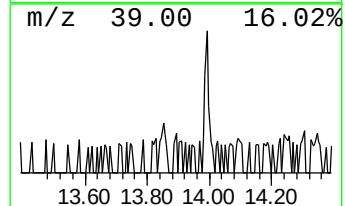
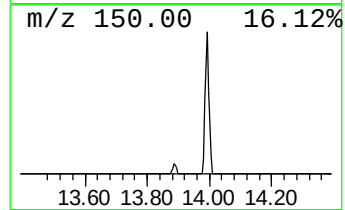
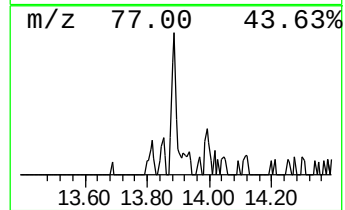
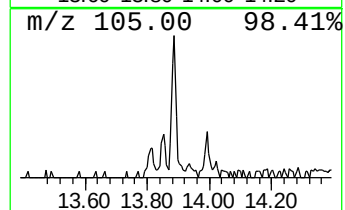
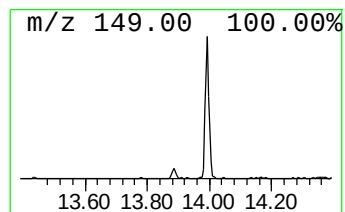
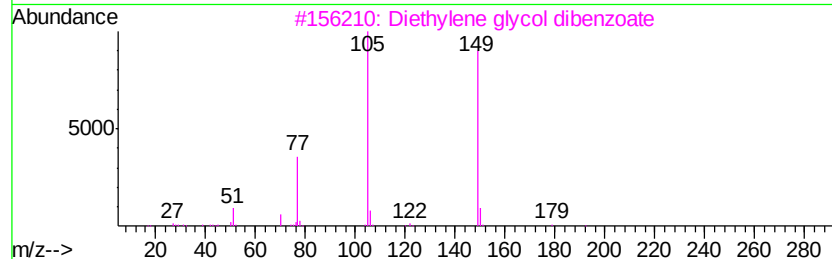
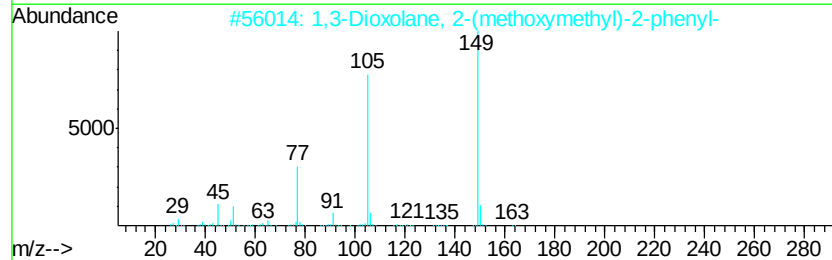
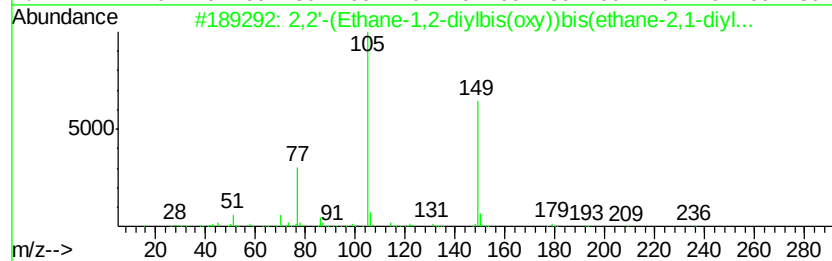
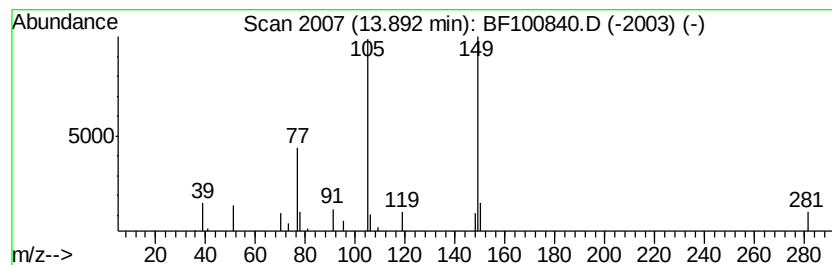
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.04 ng	20041	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	78
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
3		Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
4		Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
5		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64



Data Path : Z:\HPCHEM1\BNA_F\Data\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	6.2	ng	24937	1	6.86	79950	20.0
unknown6.62	6.62	98.9	ng	395287	1	6.86	79950	20.0
unknown9.82	9.82	3.3	ng	21193	3	9.89	128316	20.0
n-Hexadecanoic acid	11.90	12.5	ng	82079	4	11.38	131498	20.0
Tetradecanoic acid	12.68	7.3	ng	47932	4	11.38	131498	20.0
1-Heneicosanol	13.85	7.9	ng	51970	5	14.02	131761	20.0
2,2'-(Ethane-1,2-...	13.89	3.0	ng	20041	5	14.02	131761	20.0