

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
 Data File : BF096607.D
 Acq On : 10 Jul 2017 18:07
 Operator : SJ/JU
 Sample : I4101-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-16

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-BF070117.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	4.875	469	474	486	rVB	370843	534050	20.58%	2.240%
2	5.298	541	546	549	rBV	2561052	2451413	94.45%	10.282%
3	6.322	715	720	723	rBV	2402367	2525432	97.30%	10.593%
4	6.451	737	742	745	rBV	2547288	2464045	94.93%	10.335%
5	6.681	777	781	785	rBV	806905	658628	25.38%	2.763%
6	6.840	804	808	811	rBV	2137881	1882137	72.51%	7.894%
7	7.239	871	876	880	rBV	1515115	1600812	61.67%	6.714%
8	7.963	994	999	1003	rBV	1005026	897471	34.58%	3.764%
9	9.039	1177	1182	1185	rBV	2503709	2595569	100.00%	10.887%
10	9.433	1245	1249	1252	rBV	310982	248437	9.57%	1.042%
11	9.622	1272	1281	1285	rBV4	17146	33549	1.29%	0.141%
12	9.716	1291	1297	1300	rBV	916002	937182	36.11%	3.931%
13	10.163	1369	1373	1376	rVB	46137	39001	1.50%	0.164%
14	10.380	1404	1410	1413	rBV2	17892	27812	1.07%	0.117%
15	10.498	1425	1430	1438	rBV	1455688	1406734	54.20%	5.900%
16	10.633	1449	1453	1462	rBV	63034	72382	2.79%	0.304%
17	11.080	1524	1529	1531	rBV2	40428	37698	1.45%	0.158%
18	11.192	1543	1548	1551	rBV	1002050	883397	34.03%	3.705%
19	12.621	1785	1791	1796	rVB	25265	26644	1.03%	0.112%
20	12.780	1812	1818	1821	rBV	2083677	2172050	83.68%	9.110%
21	13.474	1931	1936	1940	rBV	86443	72987	2.81%	0.306%
22	13.657	1964	1967	1968	rBV	64975	54681	2.11%	0.229%
23	13.680	1968	1971	1978	rVV	233668	261423	10.07%	1.097%
24	13.733	1978	1980	1984	rVB	66841	63520	2.45%	0.266%
25	13.816	1990	1994	1998	rBV	785322	732318	28.21%	3.072%
26	13.968	2011	2020	2023	rBV5	28851	60205	2.32%	0.253%
27	14.127	2042	2047	2053	rVB4	26558	29798	1.15%	0.125%
28	14.316	2075	2079	2085	rBV3	71750	147249	5.67%	0.618%
29	14.674	2136	2140	2143	rVB	27165	29977	1.15%	0.126%
30	14.915	2177	2181	2183	rBV	27893	34767	1.34%	0.146%
31	14.939	2183	2185	2191	rVB3	34578	50395	1.94%	0.211%
32	15.210	2227	2231	2238	rBV	451345	553166	21.31%	2.320%
33	15.710	2311	2316	2323	rVB4	32372	56562	2.18%	0.237%
34	17.092	2546	2551	2560	rBV4	18907	41723	1.61%	0.175%

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Instrument :
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ClientSampleId :
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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-BF070117.M
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35	17.174	2560	2565	2573	rVB9	13828	41144	1.59%	0.173%
36	17.598	2630	2637	2645	rBV9	37543	84150	3.24%	0.353%
37	18.956	2861	2868	2876	rVB9	12768	32906	1.27%	0.138%

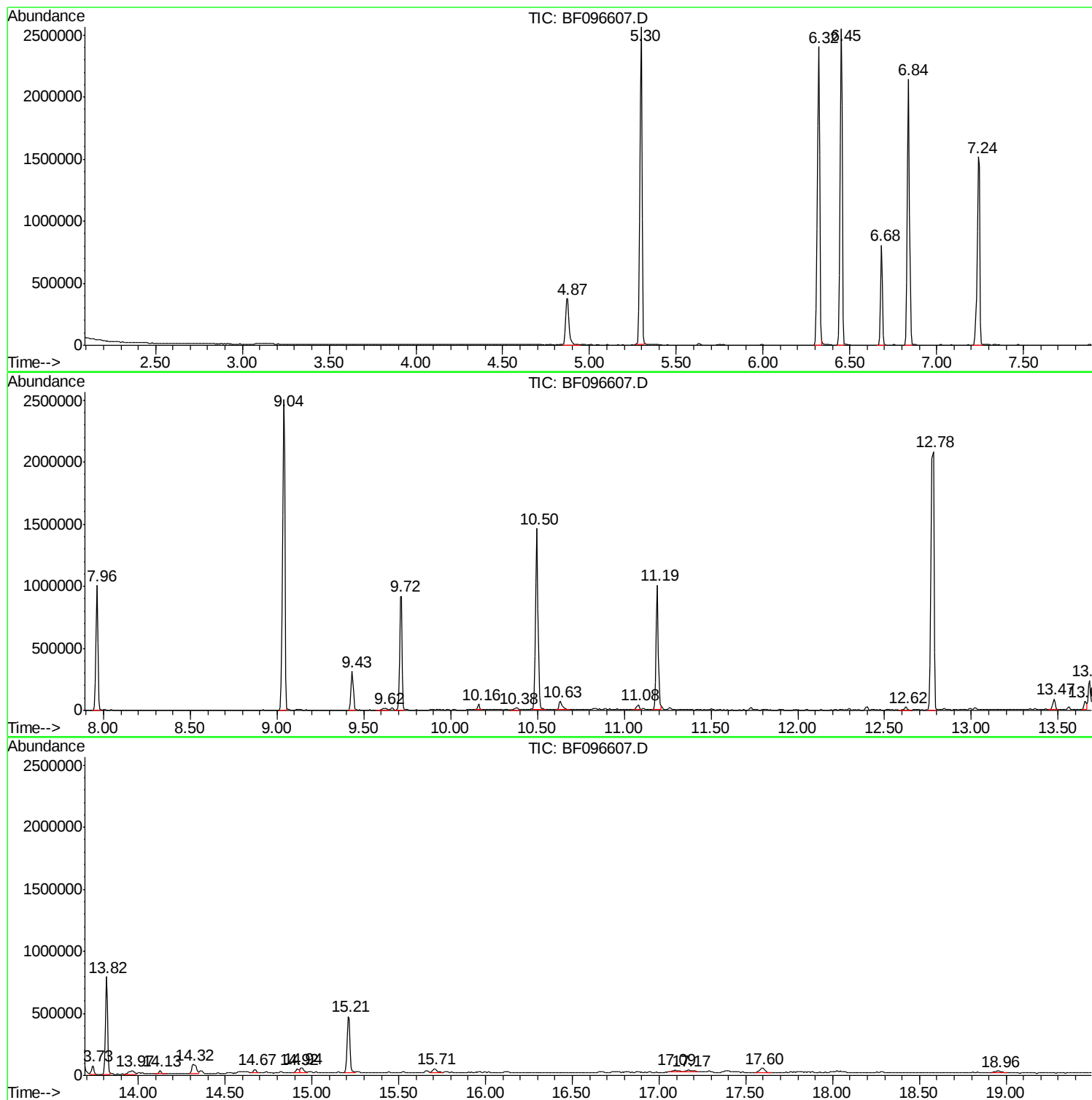
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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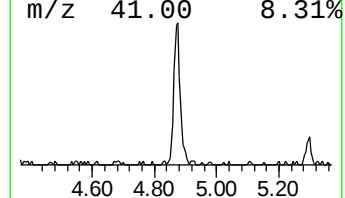
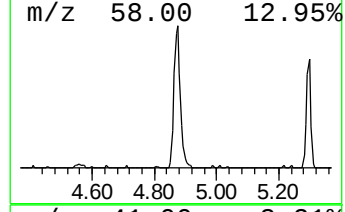
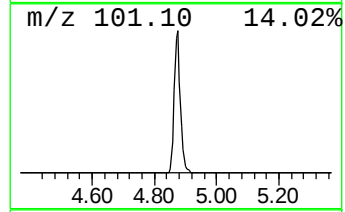
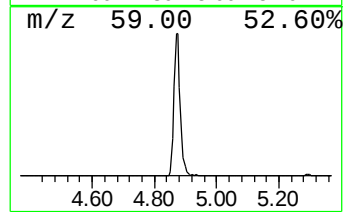
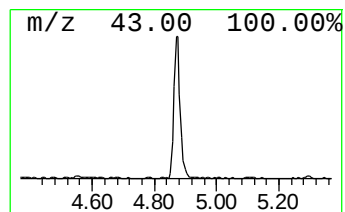
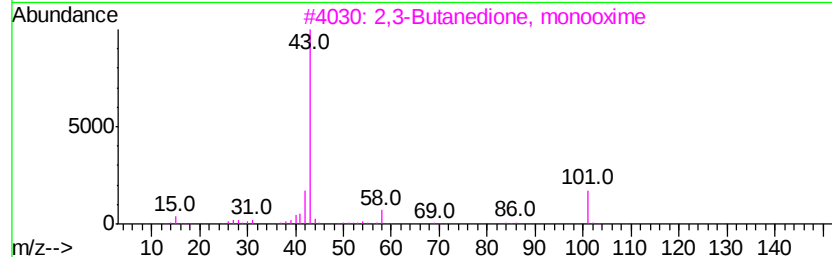
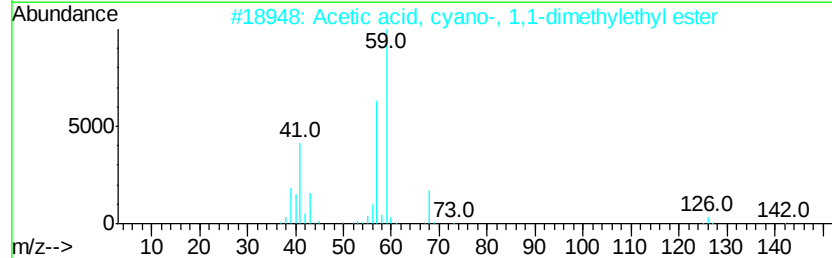
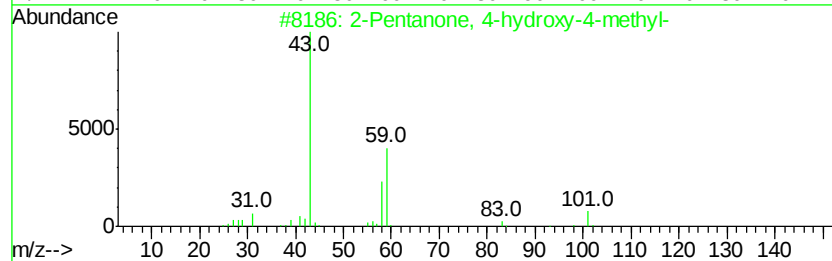
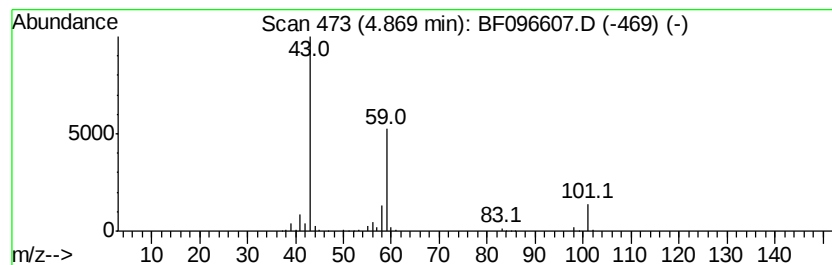
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	16.22 ng	534050	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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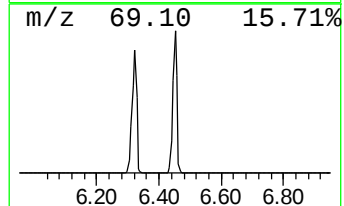
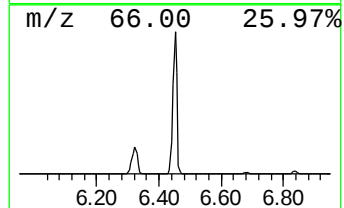
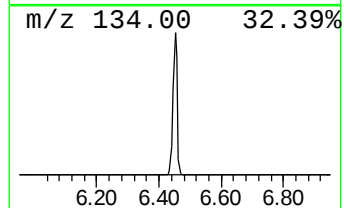
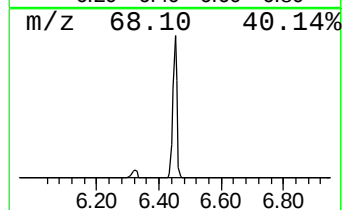
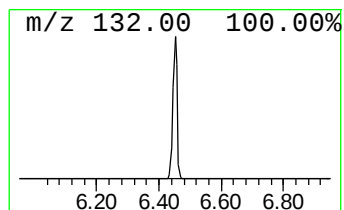
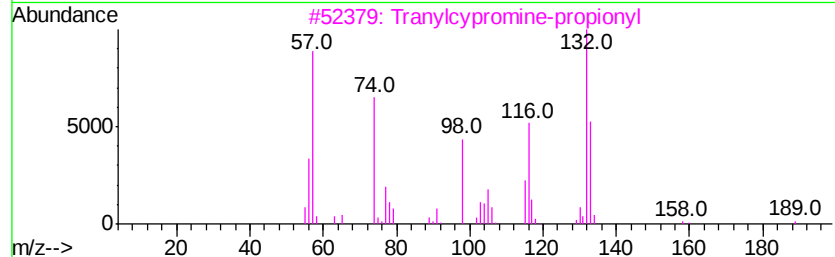
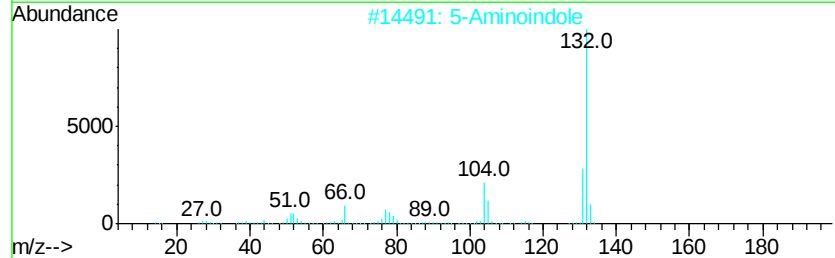
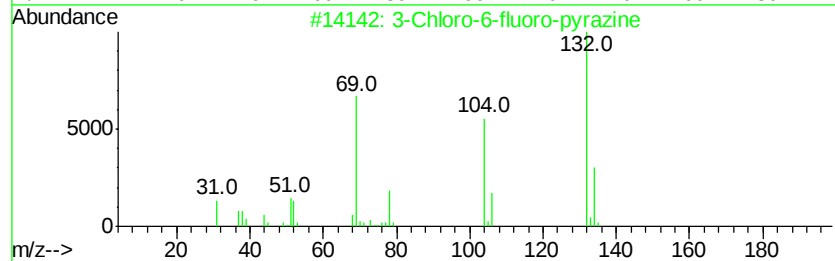
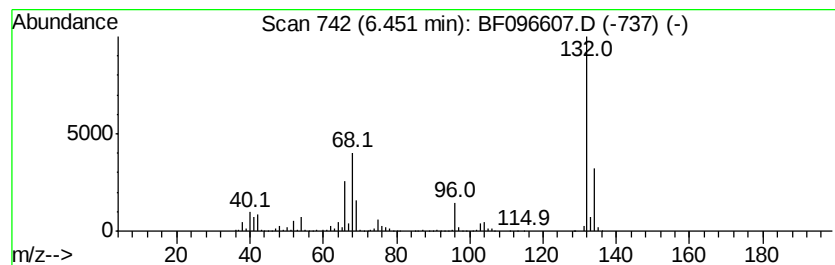
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	74.82 ng	2464050	1,4-Dichlorobenzene-d4	6.68

Hit#	of	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	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	1-Aminoindan	133	C9H11N	034698-41-4	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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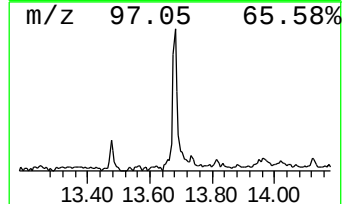
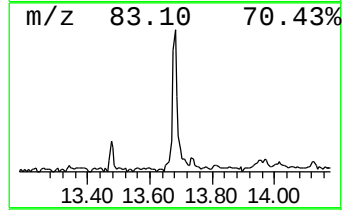
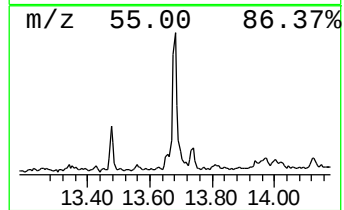
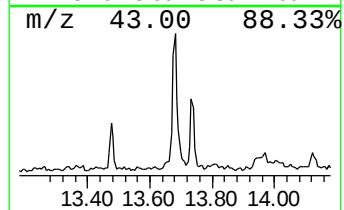
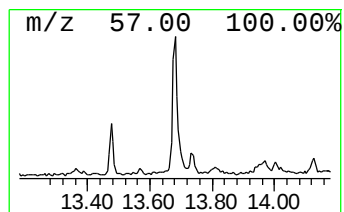
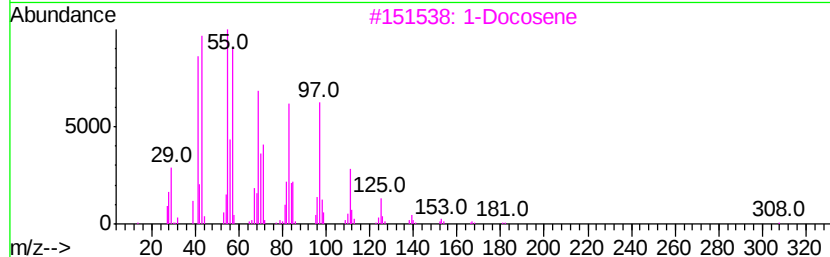
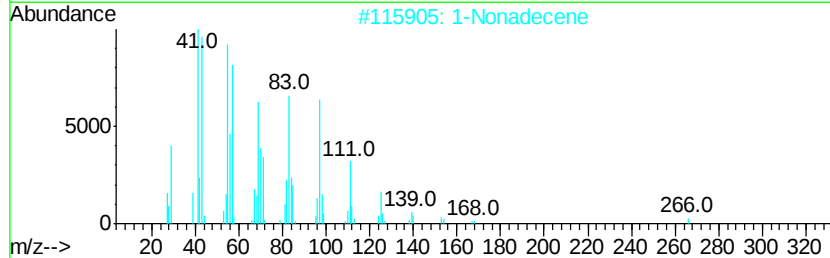
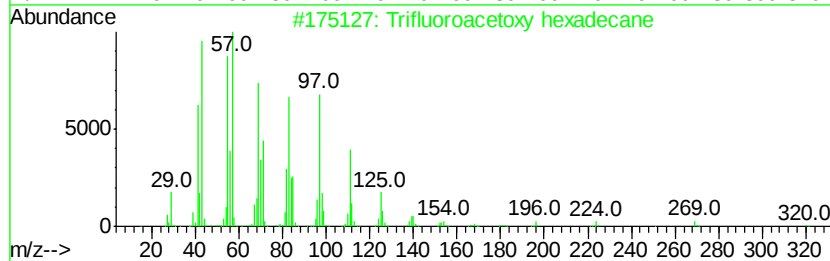
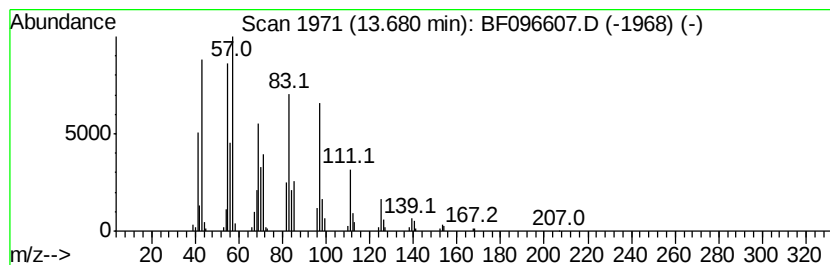
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	7.14 ng	261423	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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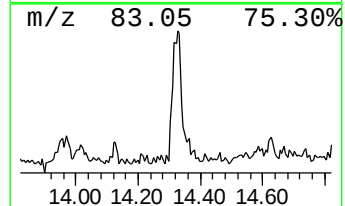
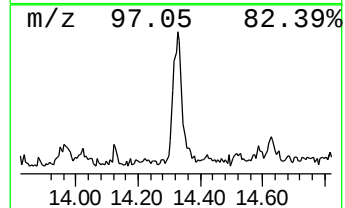
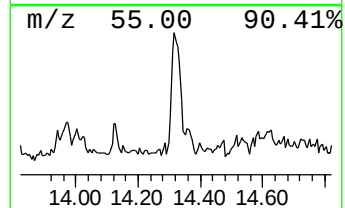
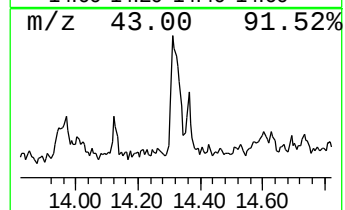
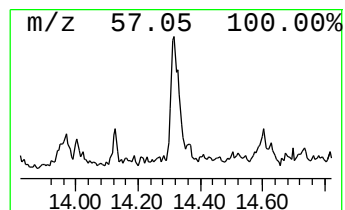
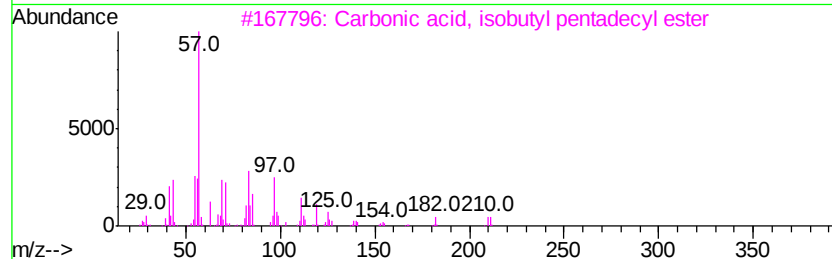
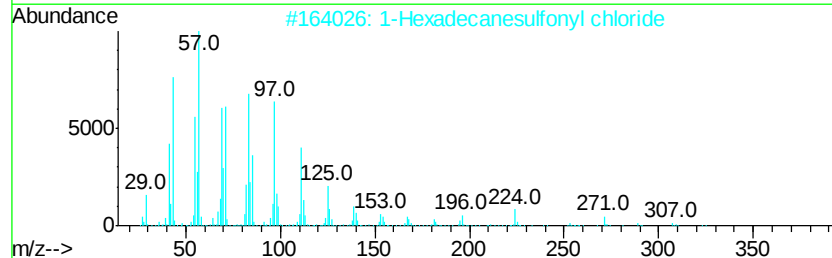
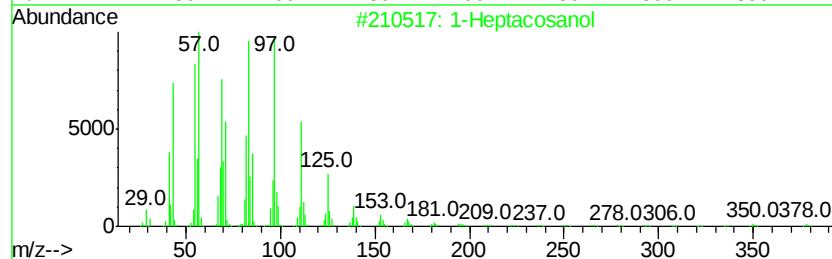
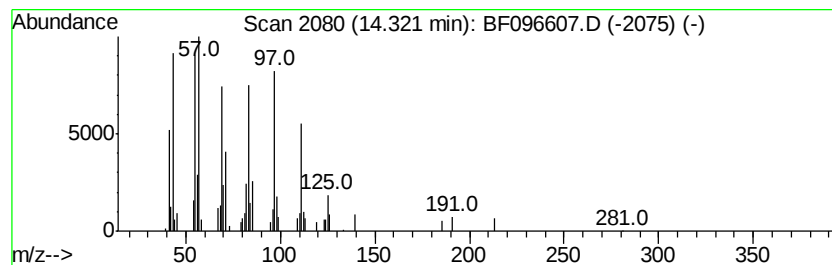
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	4.02 ng	147249	Chrysene-d12	13.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	93
2	1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1	91
3	Carbonic acid, isobutyl pentadecyl...	328 C20H40O3	1000314-61-2	90
4	Carbonic acid, heptadecyl isobutyl...	356 C22H44O3	1000314-61-4	90
5	Carbonic acid, isobutyl octadecyl...	370 C23H46O3	1000314-61-5	90



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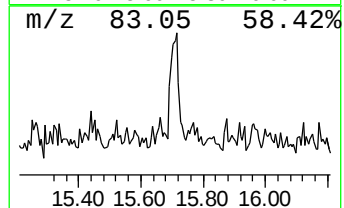
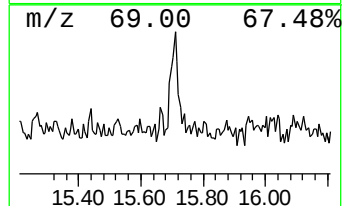
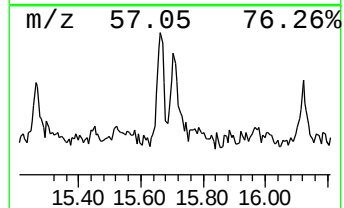
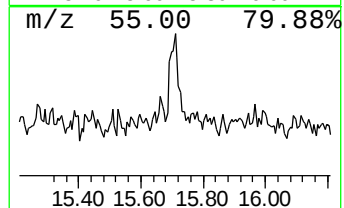
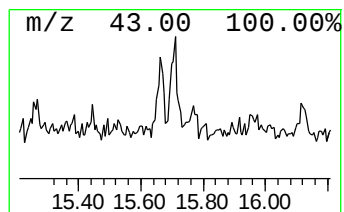
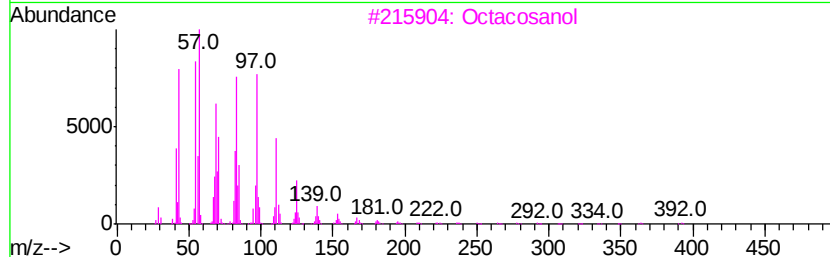
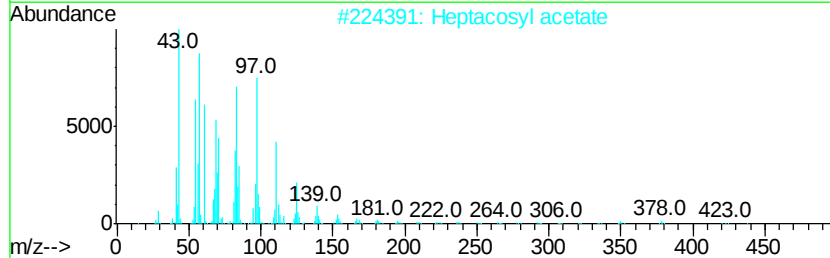
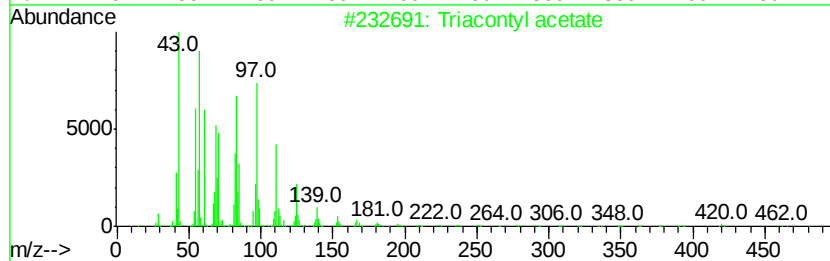
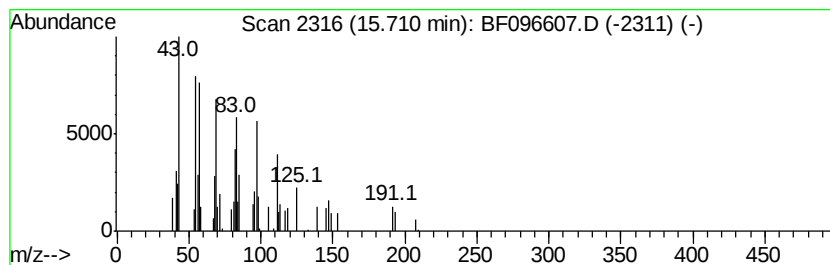
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triacontyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.71	2.05 ng	56562	Perylene-d12	15.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl acetate	480	C32H64O2	041755-58-2	86
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	72
3	Octacosanol	410	C28H58O	000557-61-9	72
4	Octacosyl acetate	452	C30H60O2	018206-97-8	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	64



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Operator : SJ/JU
Sample : I4101-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
EP-16

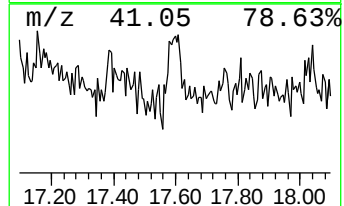
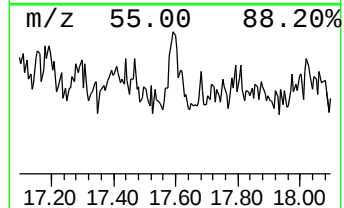
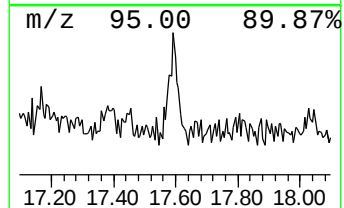
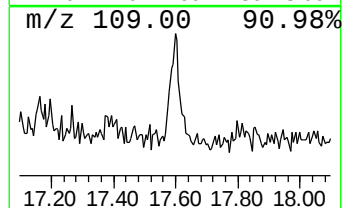
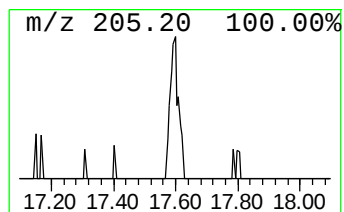
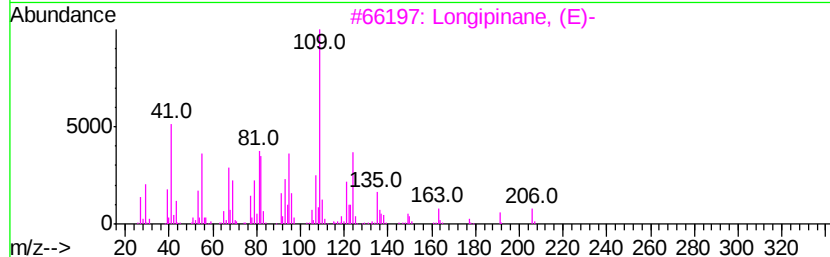
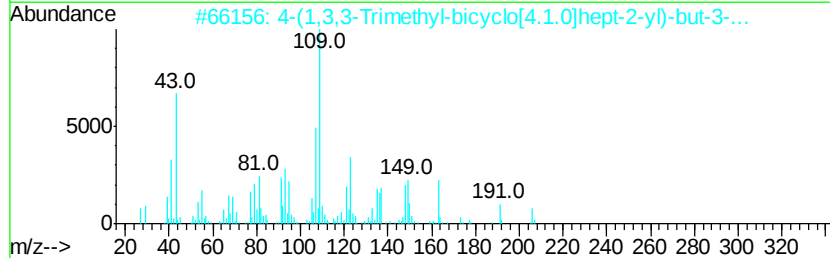
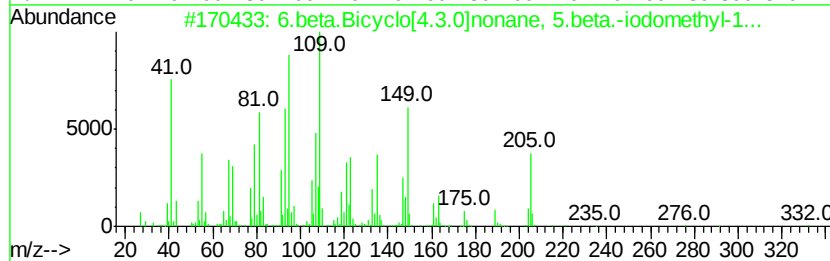
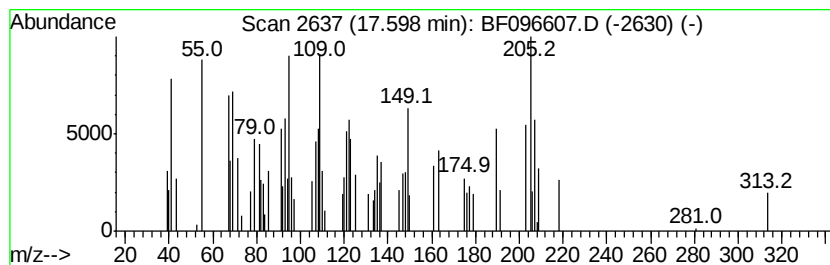
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.60 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	3.04 ng	84150	Perylene-d12	15.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6.beta.Bicvclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	46
2			4-(1,3,3-Trimethyl-bicvclo[4.1.0...	206	C14H22O	077143-31-8	38
3			Longipinane, (E)-	206	C15H26	1000156-14-5	35
4			4,7,7-Trimethylbicvclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	18
5			1,10-Dimethyl-2-methylene-trans-...	178	C13H22	1000103-97-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096607.D
Acq On : 10 Jul 2017 18:07
Operator : SJ/JU
Sample : I4101-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.87	16.2	ng	534050	1	6.68	658628	20.0
unknown6.45	6.45	74.8	ng	2464050	1	6.68	658628	20.0
Trifluoroacetoxy ...	13.68	7.1	ng	261423	5	13.82	732318	20.0
1-Heptacosanol	14.32	4.0	ng	147249	5	13.82	732318	20.0
Triacontyl acetate	15.71	2.0	ng	56562	6	15.22	553166	20.0
unknown17.60	17.60	3.0	ng	84150	6	15.22	553166	20.0