

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088157.D
 Acq On : 19 Jun 2016 2:49
 Operator : UM/SJ
 Sample : H3628-01
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-1A

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-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	1.667	6	7	15	rVB	76753	130152	5.89%	0.733%
2	1.781	15	17	51	rVB	901982	1679637	76.07%	9.459%
3	3.667	179	182	186	rVB	40674	45004	2.04%	0.253%
4	4.833	281	284	289	rBV	38843	53773	2.44%	0.303%
5	5.279	321	323	334	rBV	1025472	1172811	53.12%	6.605%
6	6.342	413	416	424	rBV	725739	889553	40.29%	5.010%
7	6.456	424	426	429	rBV	1902998	1721642	77.98%	9.696%
8	6.685	444	446	448	rBV	599438	504549	22.85%	2.841%
9	6.845	457	460	462	rVB	1556210	1774512	80.37%	9.993%
10	7.256	493	496	498	rBV	1271382	1320004	59.78%	7.434%
11	7.965	556	558	561	rBV	429944	587513	26.61%	3.309%
12	8.102	567	570	575	rBV	12379	25157	1.14%	0.142%
13	8.250	581	583	587	rVB3	24593	27595	1.25%	0.155%
14	8.970	642	646	650	rBV3	16282	33759	1.53%	0.190%
15	9.050	650	653	655	rBV	2423165	2207926	100.00%	12.434%
16	9.451	686	688	689	rBV	23322	24494	1.11%	0.138%
17	9.668	704	707	709	rVB2	20862	31205	1.41%	0.176%
18	9.725	709	712	714	rBV	487720	583887	26.45%	3.288%
19	9.896	725	727	730	rBV2	20788	35426	1.60%	0.200%
20	10.125	742	747	748	rBV2	16332	40756	1.85%	0.230%
21	10.159	748	750	752	rVB	34254	35296	1.60%	0.199%
22	10.342	763	766	768	rBV	53609	97419	4.41%	0.549%
23	10.376	768	769	773	rVB	23662	30858	1.40%	0.174%
24	10.513	778	781	783	rVV	884157	1108019	50.18%	6.240%
25	10.582	785	787	790	rVV2	18682	32696	1.48%	0.184%
26	10.628	790	791	795	rVB	53785	73758	3.34%	0.415%
27	11.096	829	832	834	rBV2	21287	40889	1.85%	0.230%
28	11.199	839	841	843	rBV	626185	521922	23.64%	2.939%
29	11.748	887	889	892	rBV3	49943	72180	3.27%	0.406%
30	11.942	904	906	911	rVB	13555	24600	1.11%	0.139%
31	12.685	968	971	973	rBV	23199	30755	1.39%	0.173%
32	12.788	977	980	982	rBV	1538558	1834002	83.06%	10.328%
33	13.359	1027	1030	1032	rBV	24091	35429	1.60%	0.200%
34	13.714	1059	1061	1067	rVB2	22490	36893	1.67%	0.208%

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Integration Parameters: rteint.p
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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.828	1069	1071	1074	rBV	531754	501497	22.71%	2.824%
36	15.211	1189	1192	1200	rVB	311757	391215	17.72%	2.203%

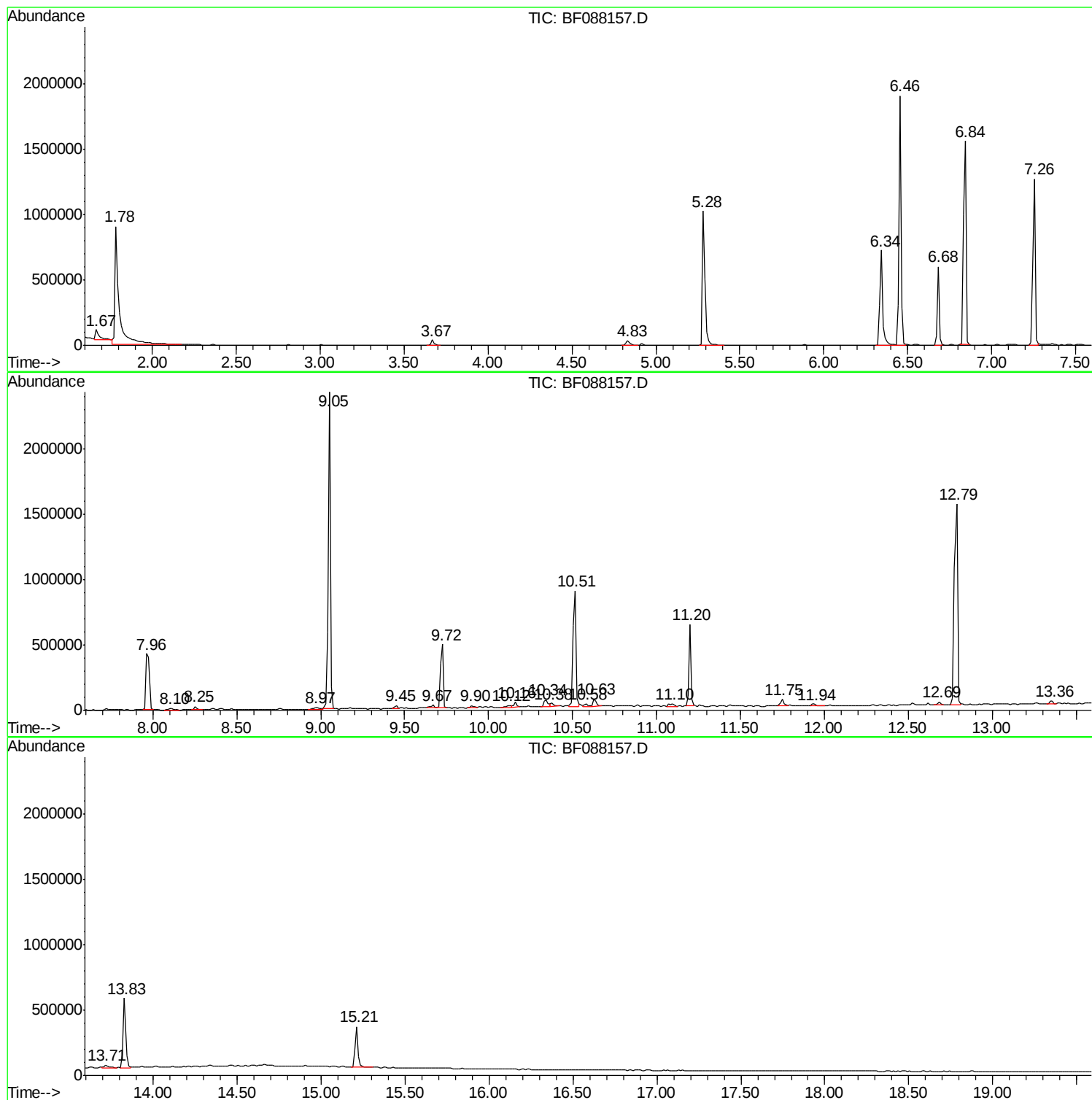
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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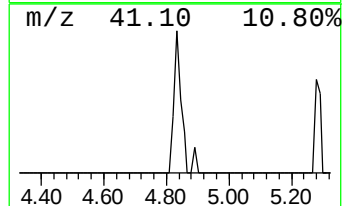
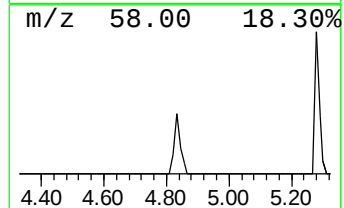
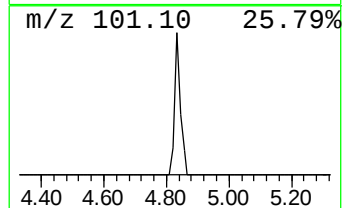
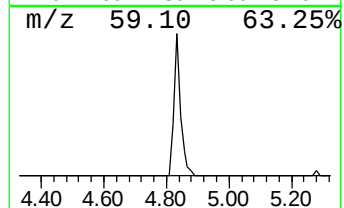
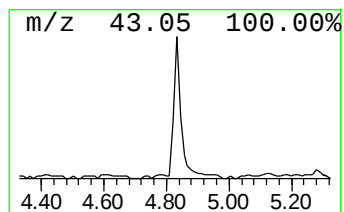
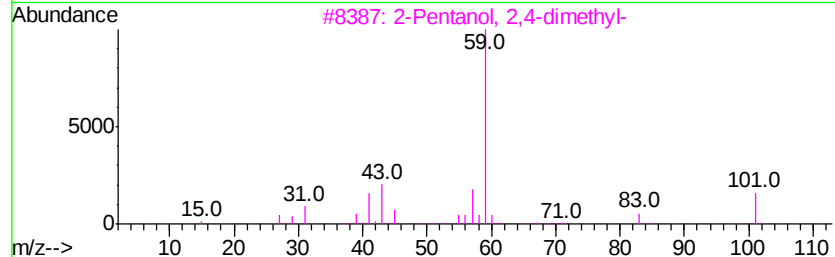
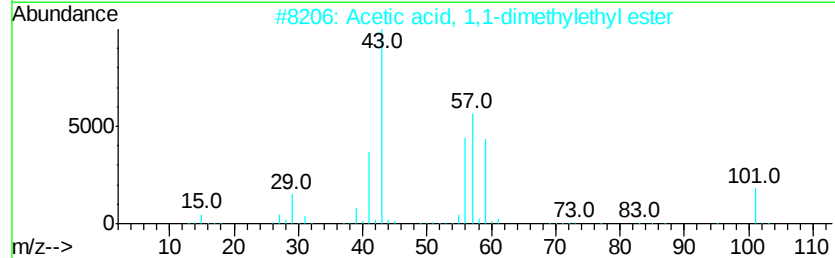
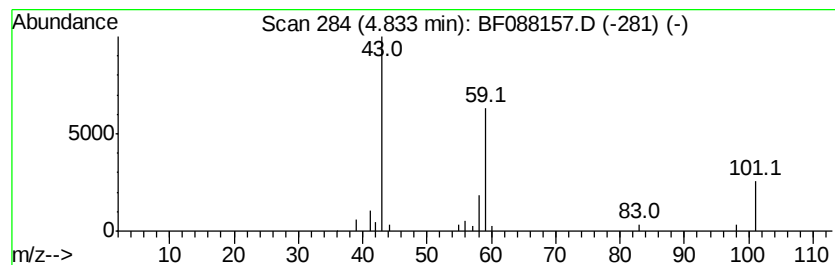
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.13 ng	53773	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	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25



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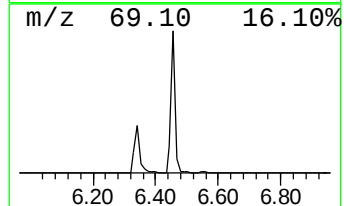
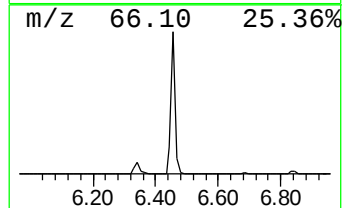
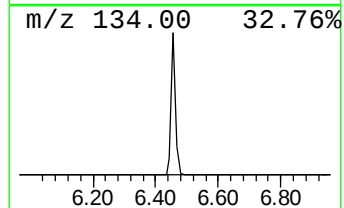
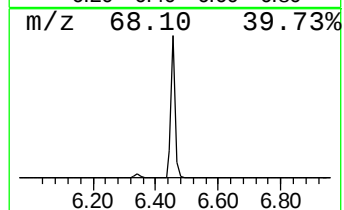
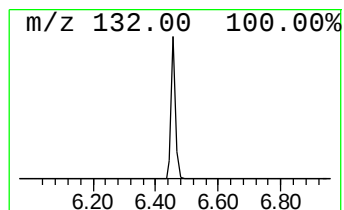
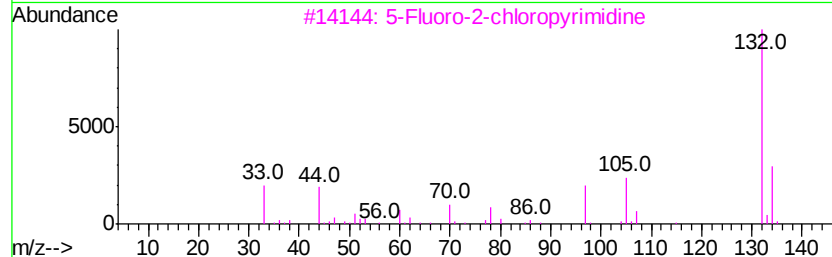
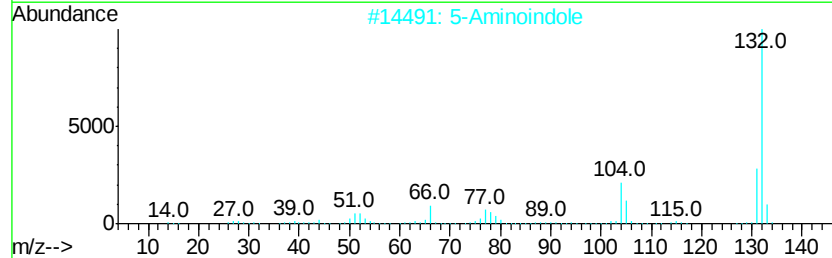
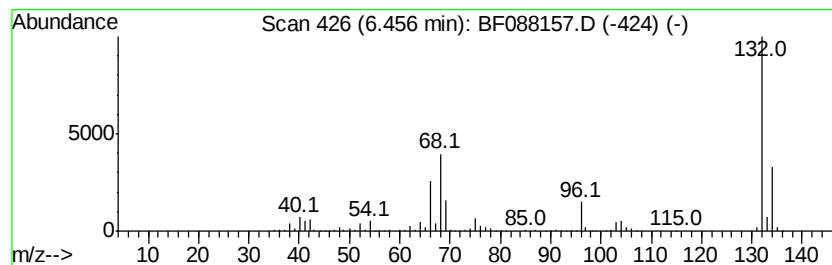
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	68.24 ng	1721640	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	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4	Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1	Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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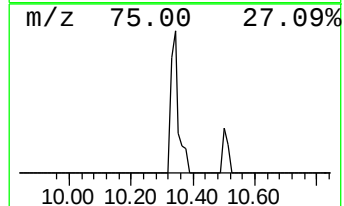
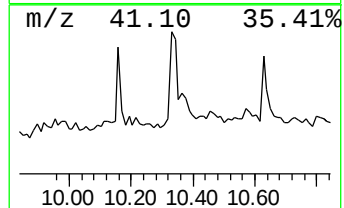
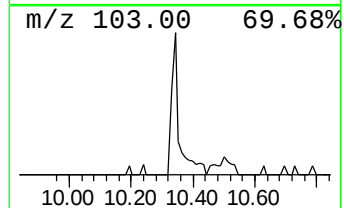
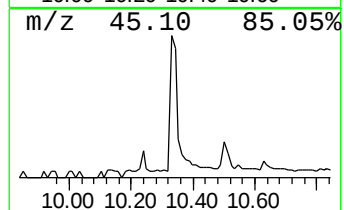
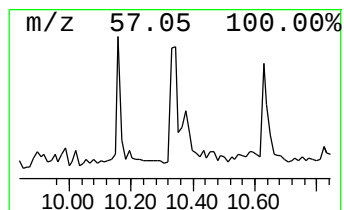
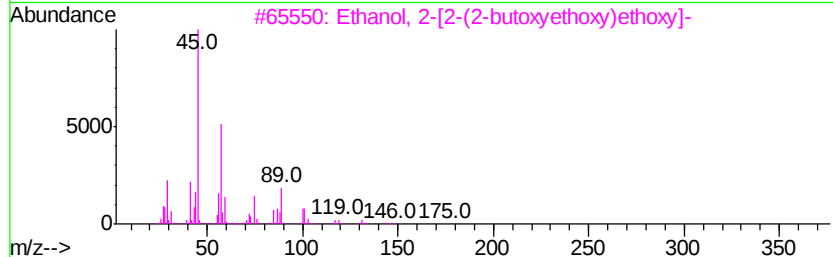
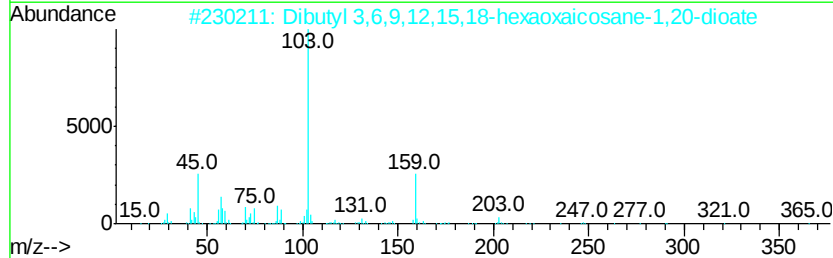
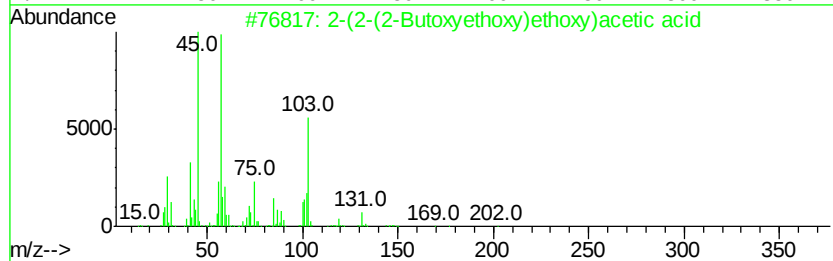
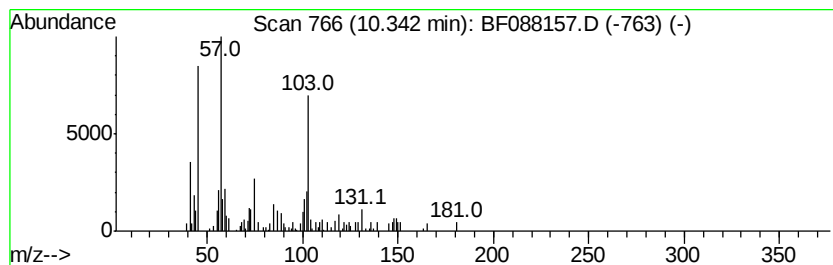
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-(2-(2-Butoxyethoxy)ethoxy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	3.34 ng	97419	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(2-(2-Butoxyethoxy)ethoxy)acet...	220	C10H20O5	1000366-77-1	91
2		Dibutyl 3,6,9,12,15,18-hexaoxaic...	466	C22H42O10	1000366-80-0	53
3		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4		Butyl 2-(2-(2-butoxyethoxy)ethox...	276	C14H28O5	1000366-77-4	47
5		Ethyl 2-(2-(2-butoxyethoxy)ethox...	248	C12H24O5	1000366-77-7	47



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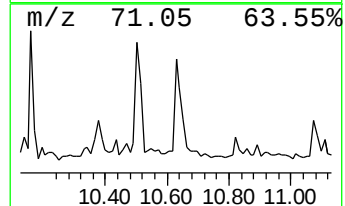
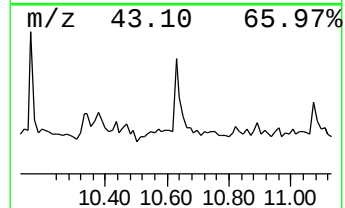
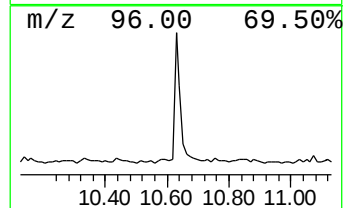
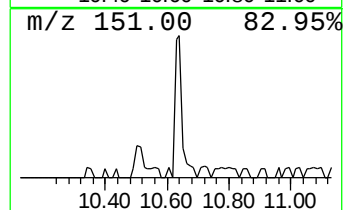
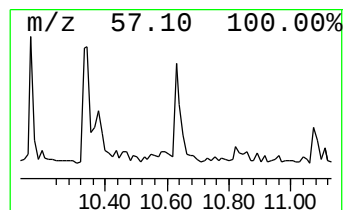
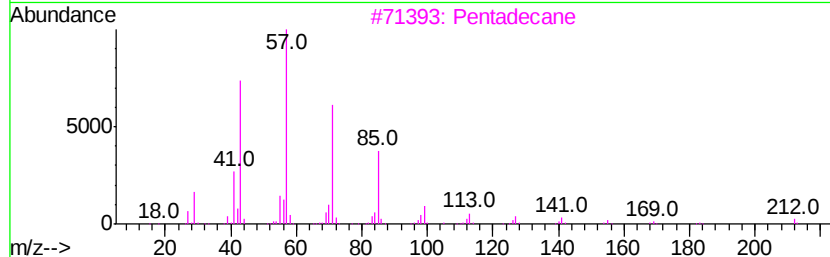
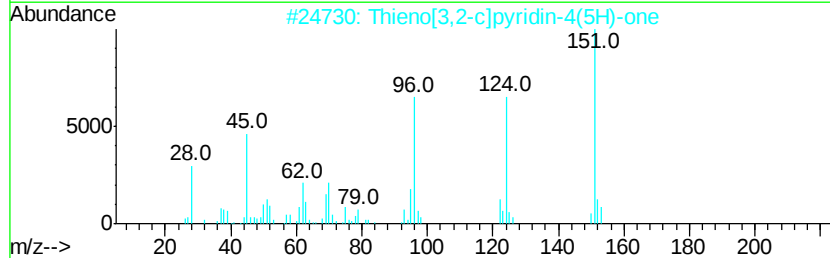
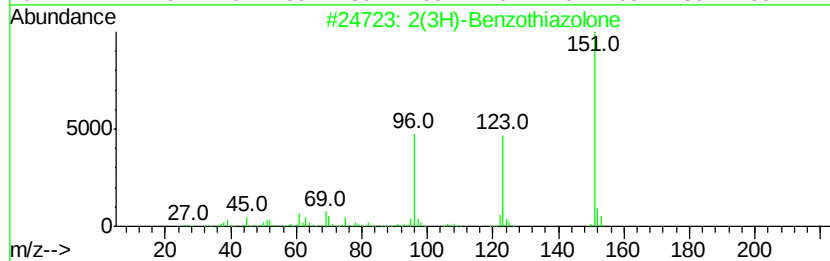
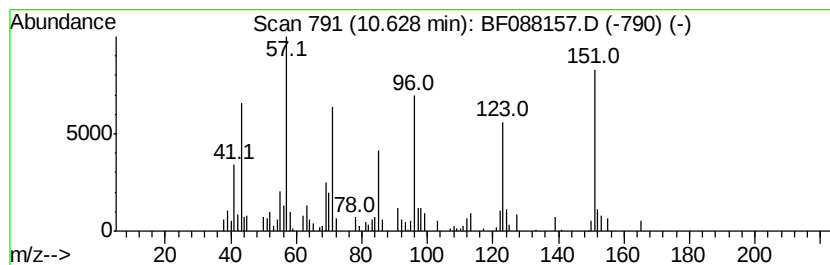
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.63 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.63	2.83 ng	73758	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	49
2	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	43
3	Pentadecane	212	C15H32	000629-62-9	22
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	18
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	14



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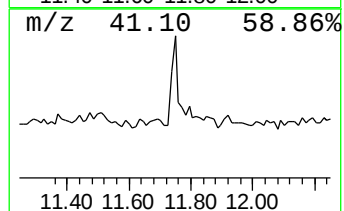
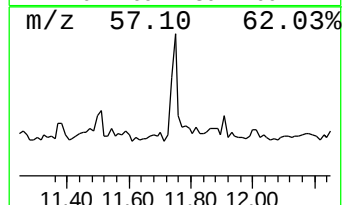
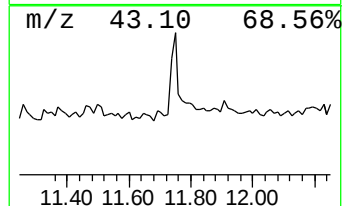
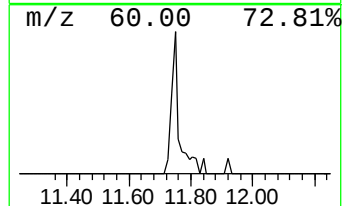
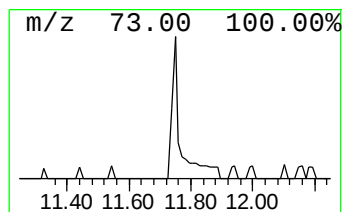
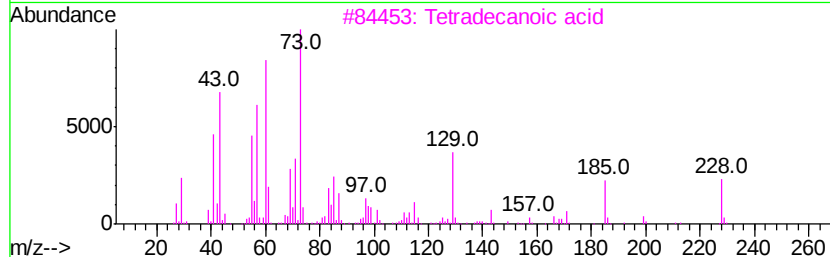
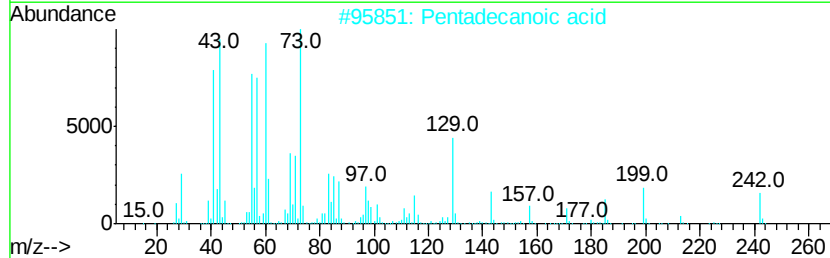
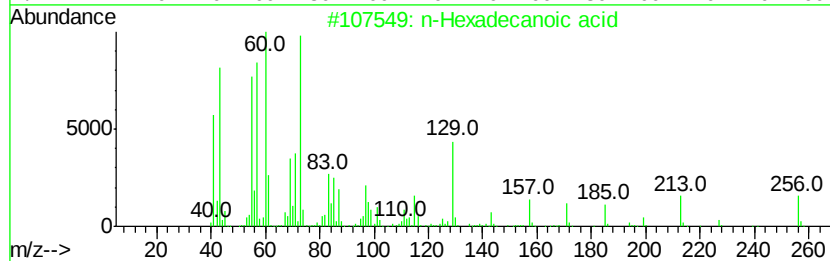
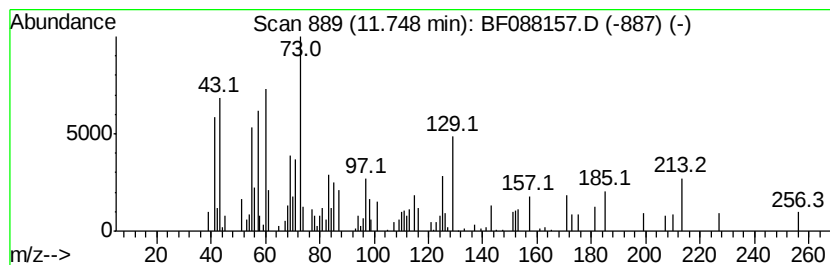
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.77 ng	72180	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	52
5	Undecanoic acid	186	C11H22O2	000112-37-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	2.1	ng	53773	1	6.68	504549	20.0
unknown6.46	6.46	68.2	ng	1721640	1	6.68	504549	20.0
2-(2-(2-Butoxyeth...	10.34	3.3	ng	97419	3	9.72	583887	20.0
unknown10.63	10.63	2.8	ng	73758	4	11.20	521922	20.0
n-Hexadecanoic acid	11.75	2.8	ng	72180	4	11.20	521922	20.0