

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
 Data File : BP001045.D
 Acq On : 15 Nov 2019 17:55
 Operator : JU
 Sample : K5832-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 10-(2-4)

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:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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	2.328	34	41	51	rVB	367172	543599	9.36%	1.146%
2	5.728	613	619	631	rBV	372684	551184	9.49%	1.162%
3	6.299	710	716	721	rBV	2709227	3272129	56.32%	6.900%
4	7.810	965	973	985	rBV	2769266	3676185	63.27%	7.752%
5	8.004	999	1006	1011	rBV	3103191	3748053	64.51%	7.903%
6	8.363	1062	1067	1072	rVB	1227118	1398522	24.07%	2.949%
7	8.604	1102	1108	1113	rBV	2813751	3112463	53.57%	6.563%
8	9.240	1209	1216	1220	rBV	1839159	2232099	38.42%	4.707%
9	10.393	1406	1412	1417	rBV	1516049	1791986	30.84%	3.779%
10	12.169	1706	1714	1719	rBV	4040600	5044165	86.82%	10.636%
11	12.840	1818	1828	1834	rBV	271487	316423	5.45%	0.667%
12	13.257	1892	1899	1905	rBV	1846724	2289860	39.41%	4.829%
13	14.545	2111	2118	2131	rBV	2818916	3608683	62.11%	7.609%
14	15.651	2300	2306	2310	rBV	2099917	2437998	41.96%	5.141%
15	15.786	2326	2329	2335	rVB	74247	81581	1.40%	0.172%
16	16.528	2449	2455	2464	rBV2	164084	270533	4.66%	0.570%
17	17.386	2597	2601	2606	rVB	108644	127643	2.20%	0.269%
18	17.616	2637	2640	2647	rBV3	45625	64214	1.11%	0.135%
19	17.692	2649	2653	2657	rVB	120993	143327	2.47%	0.302%
20	17.927	2687	2693	2697	rBV	5579492	5810141	100.00%	12.252%
21	18.298	2751	2756	2759	rBV2	47287	66777	1.15%	0.141%
22	18.745	2828	2832	2835	rBV	71435	77480	1.33%	0.163%
23	19.169	2900	2904	2915	rBV2	214058	386950	6.66%	0.816%
24	19.286	2918	2924	2928	rVV	2229837	2451779	42.20%	5.170%
25	19.316	2928	2929	2940	rVB2	97060	107466	1.85%	0.227%
26	19.574	2970	2973	2977	rVB	119059	121542	2.09%	0.256%
27	19.969	3036	3040	3043	rBV	136335	162702	2.80%	0.343%
28	20.345	3100	3104	3110	rVB	155625	180127	3.10%	0.380%
29	20.427	3114	3118	3123	rBV	223551	243846	4.20%	0.514%
30	20.574	3139	3143	3146	rBV	92357	146649	2.52%	0.309%
31	20.745	3168	3172	3177	rBV	144620	194765	3.35%	0.411%
32	20.921	3199	3202	3209	rVB	57183	72620	1.25%	0.153%
33	20.992	3211	3214	3217	rVV	58084	68335	1.18%	0.144%
34	21.068	3221	3227	3238	rVB	1656591	2302909	39.64%	4.856%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
10-(2-4)

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

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35	21.186	3243	3247	3253	rVB	119424	182431	3.14%	0.385%
36	21.692	3330	3333	3339	rVB2	83304	136638	2.35%	0.288%

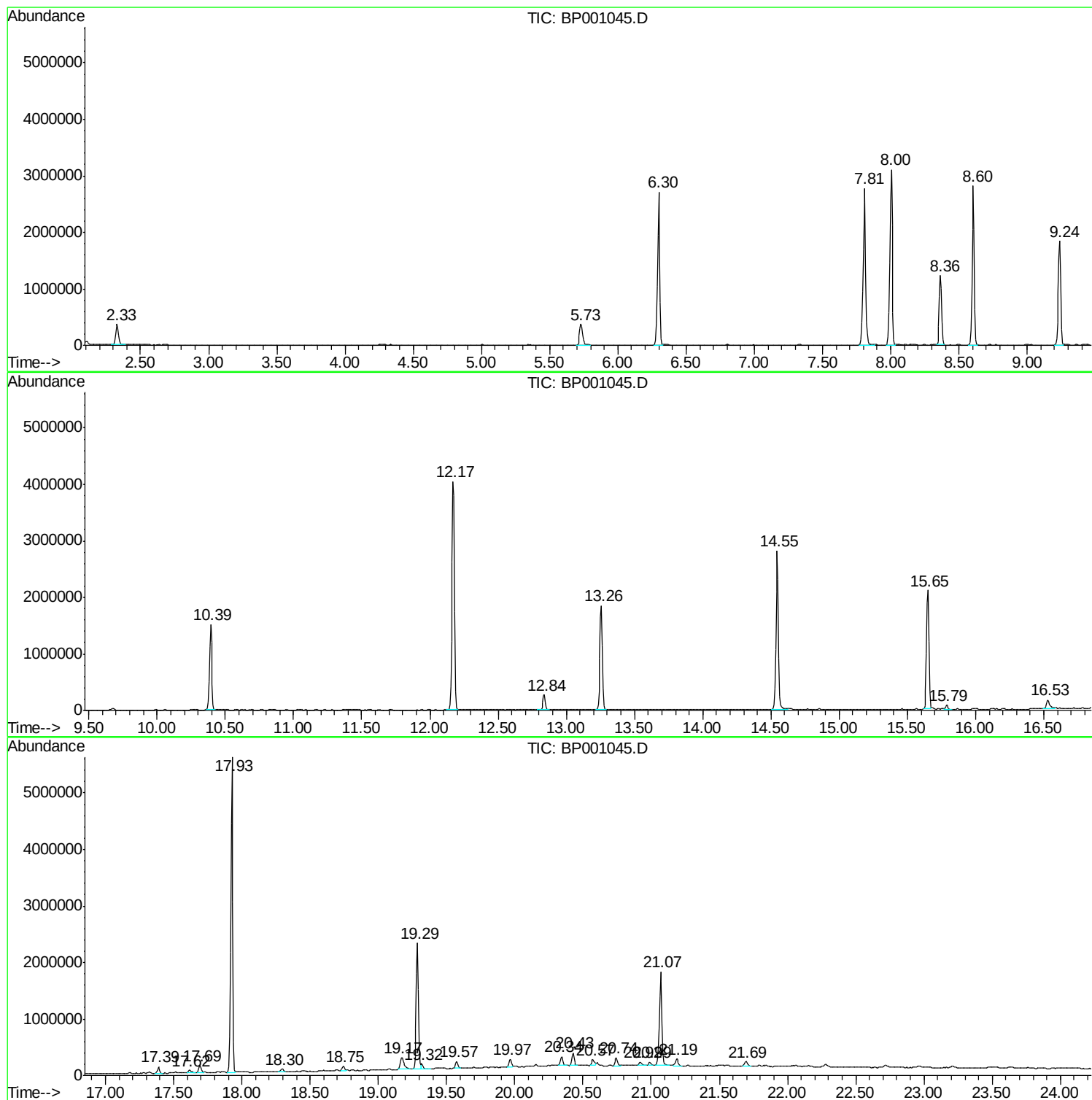
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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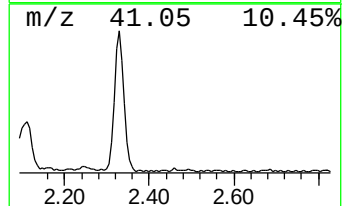
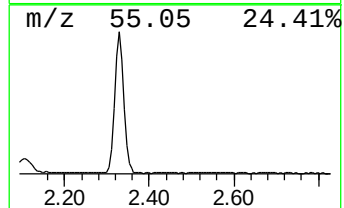
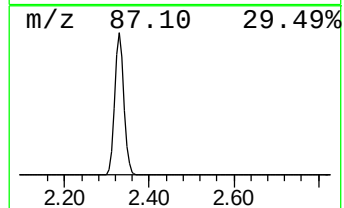
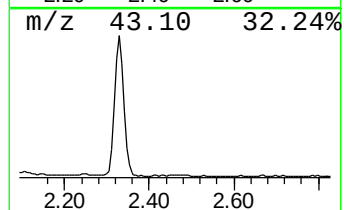
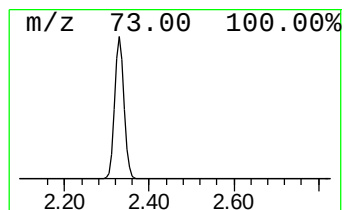
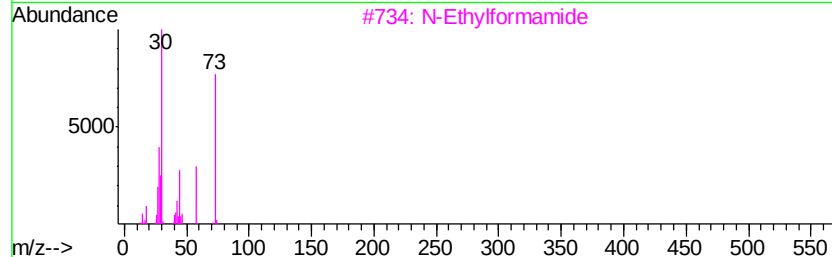
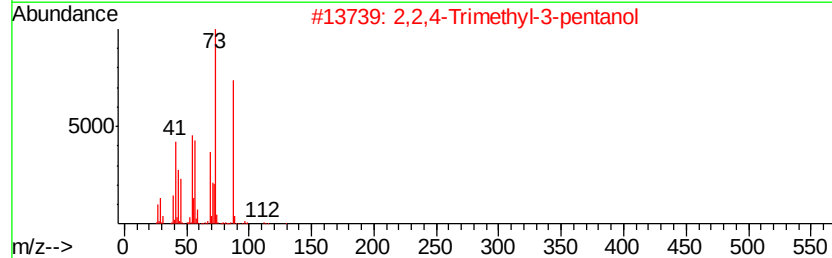
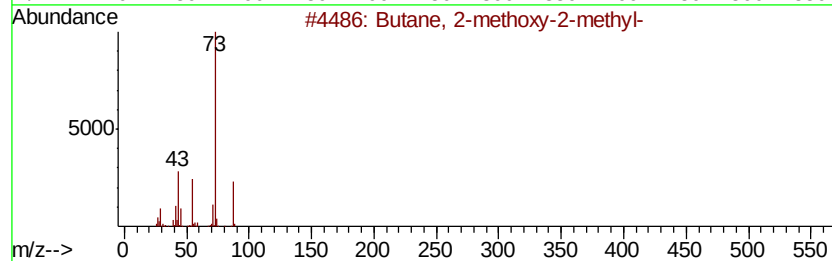
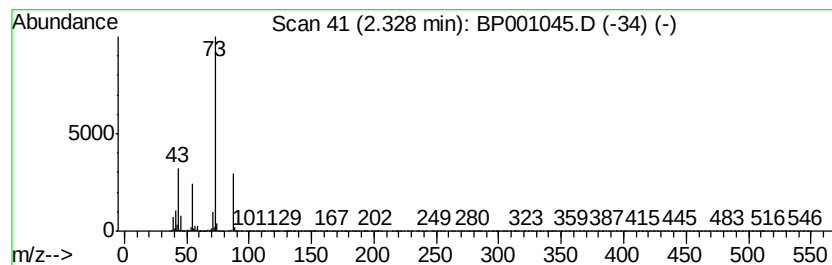
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	7.77 ng	543599	1,4-Dichlorobenzene-d4	8.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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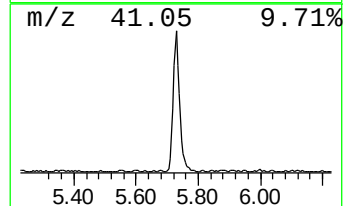
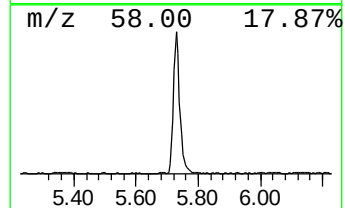
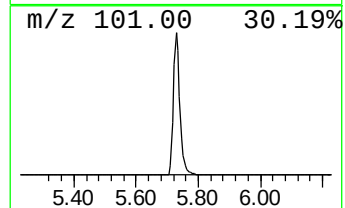
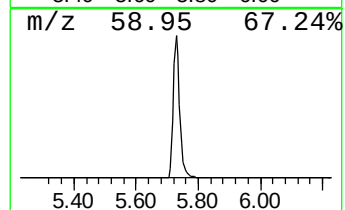
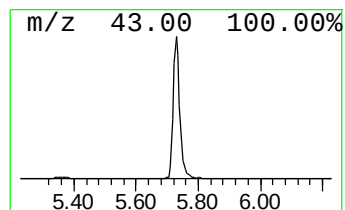
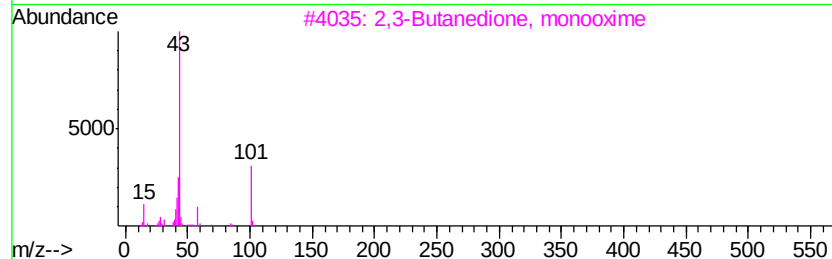
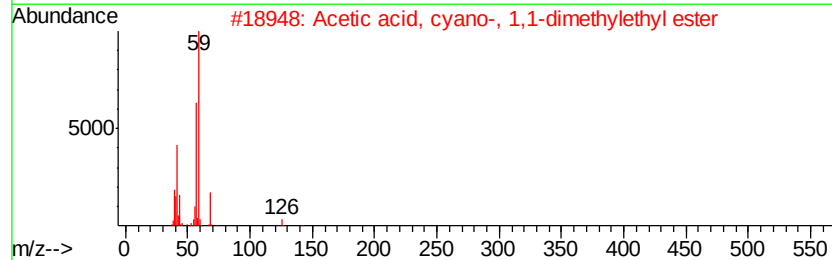
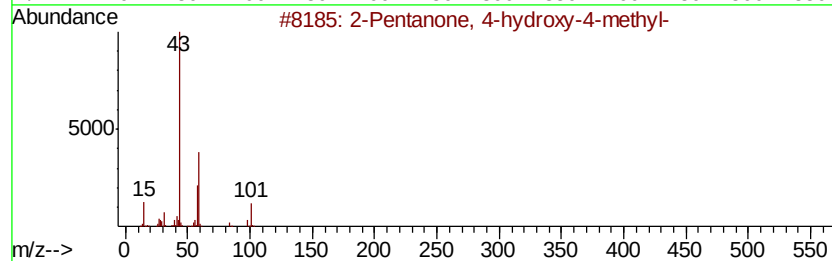
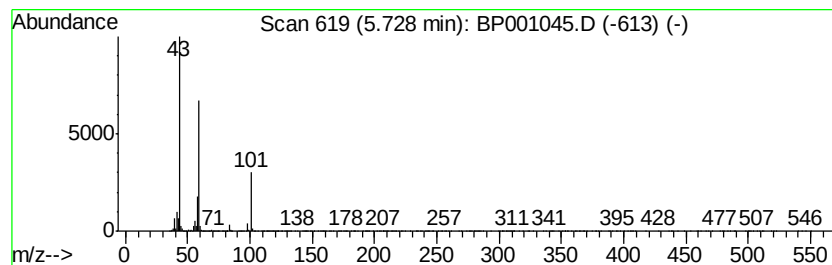
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.73 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	7.88 ng	551184	1,4-Dichlorobenzene-d4	8.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
4	Acetone	58	C3H6O	000067-64-1	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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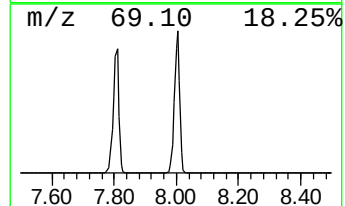
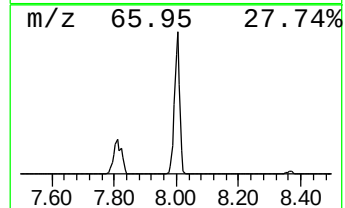
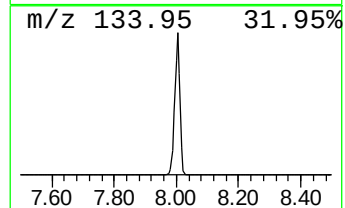
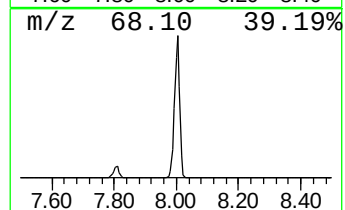
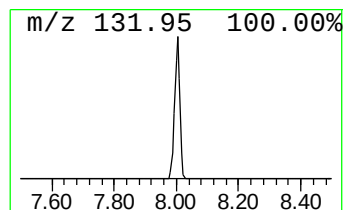
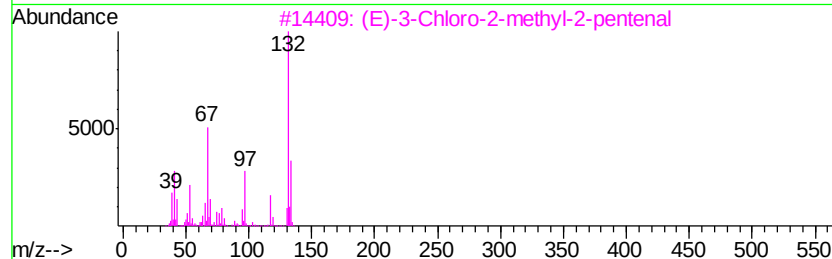
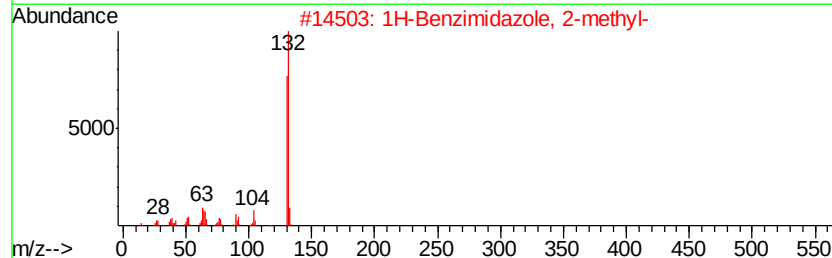
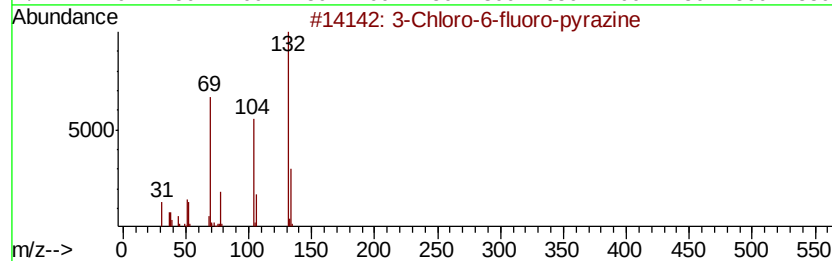
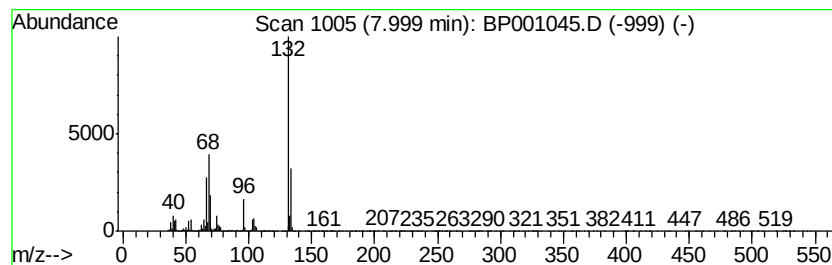
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.00	53.60 ng	3748050	1,4-Dichlorobenzene-d4	8.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
3	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	16
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
5	Tranlylcypromine-propionyl			189	C12H15NO	1000123-86-3	12



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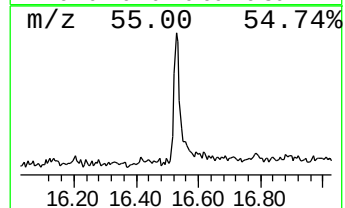
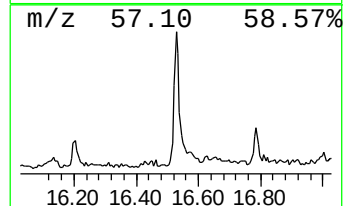
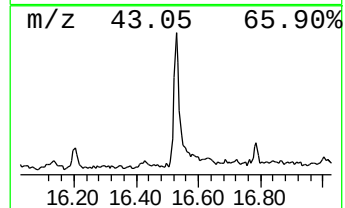
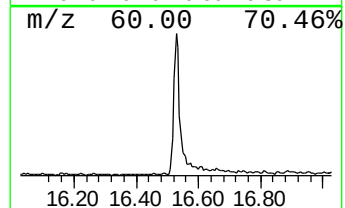
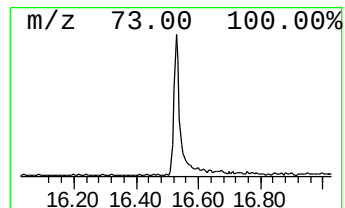
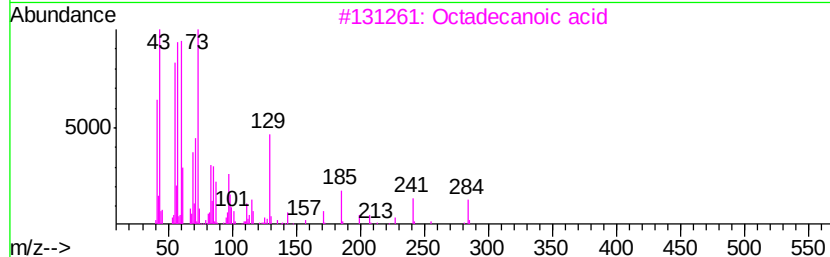
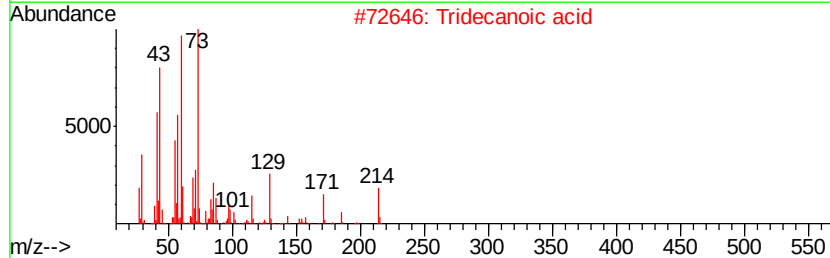
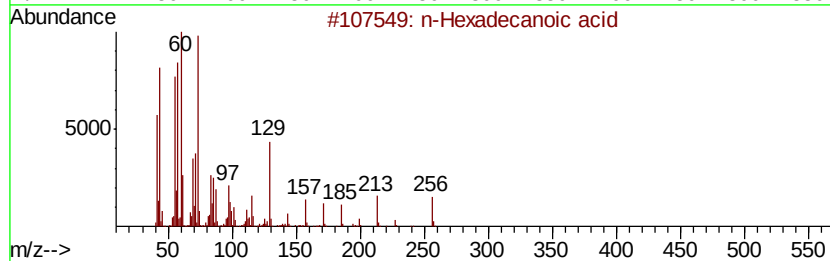
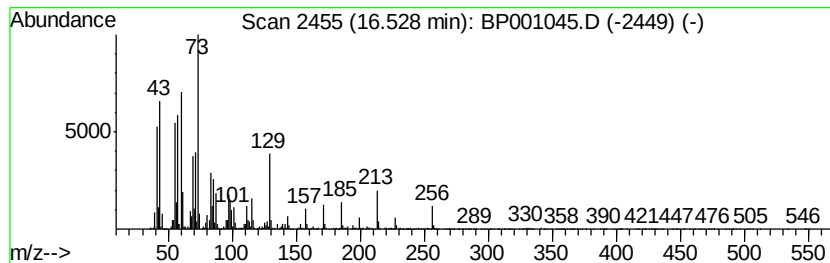
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.22 ng	270533	Phenanthrene-d10	15.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Octadecanoic acid	284	C18H36O2	000057-11-4	81
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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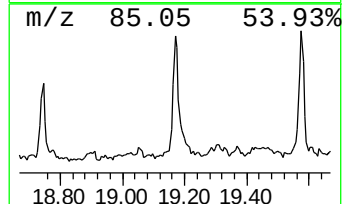
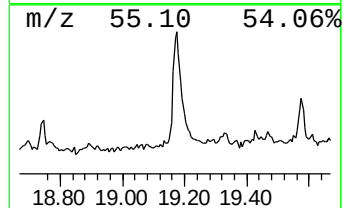
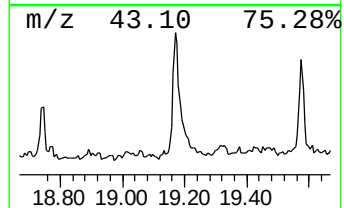
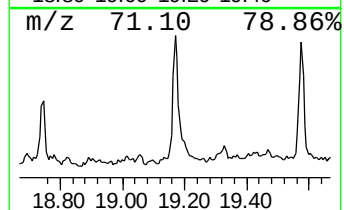
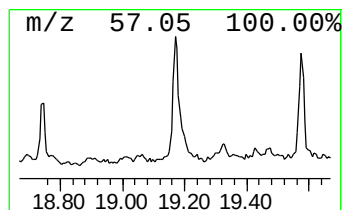
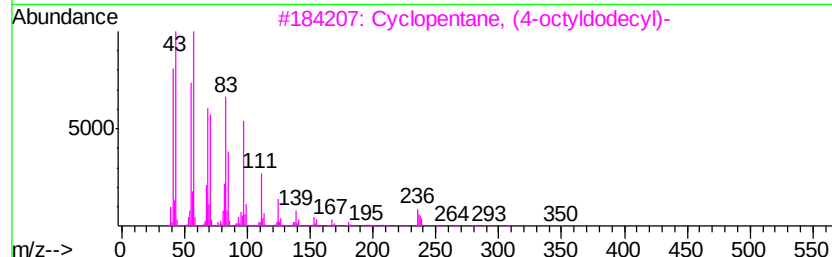
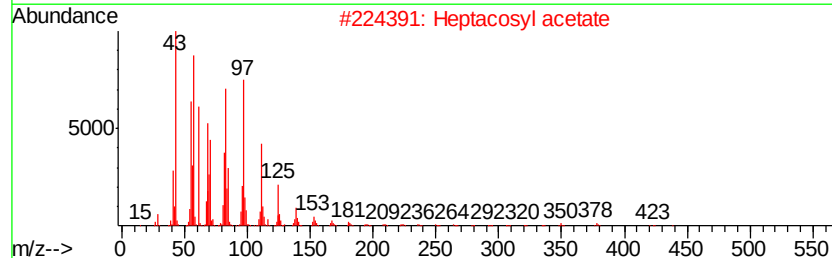
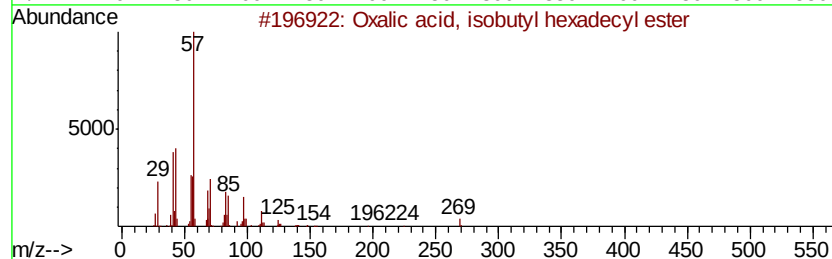
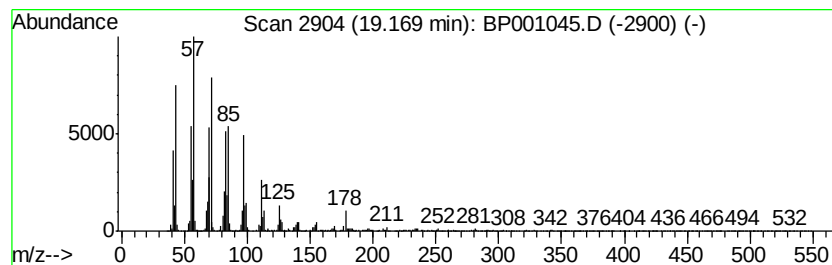
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	3.16 ng	386950	Chrysene-d12	19.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Heptacosyl acetate	438	C29H58O2	1000351-78-2	87
3		Cyclopentane, (4-octyldecyl)-	350	C25H50	005638-09-5	83
4		Eicosane	282	C20H42	000112-95-8	64
5		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	60



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Sample : K5832-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

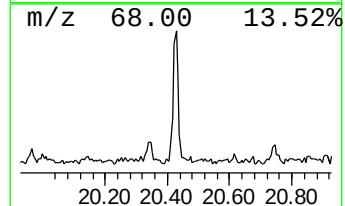
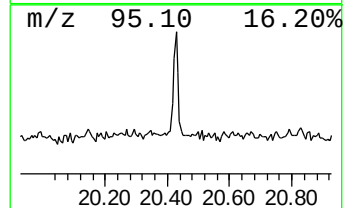
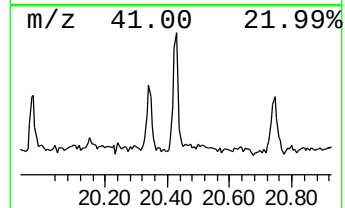
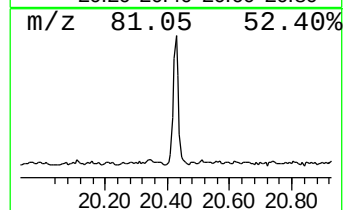
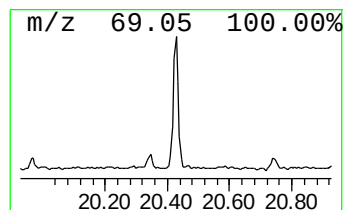
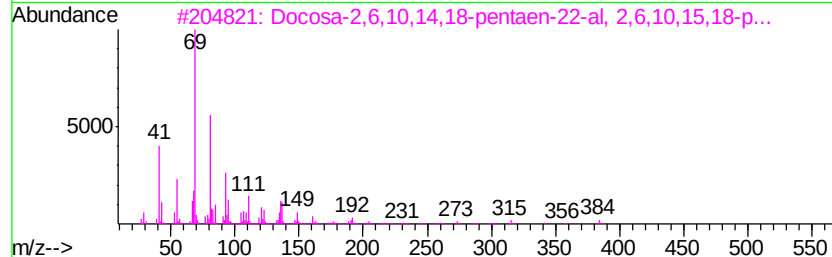
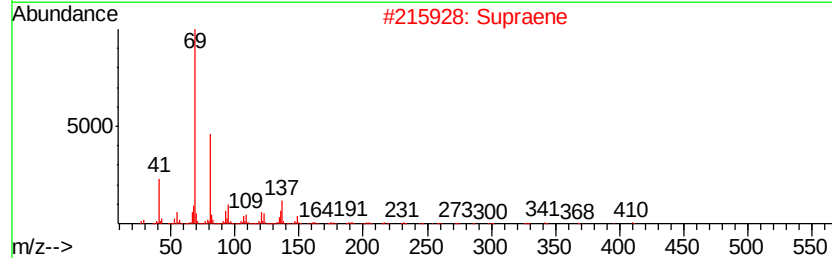
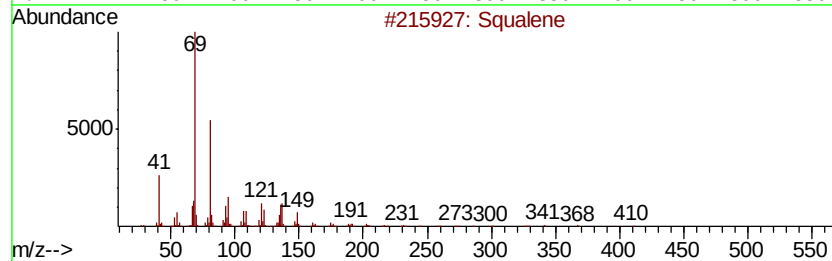
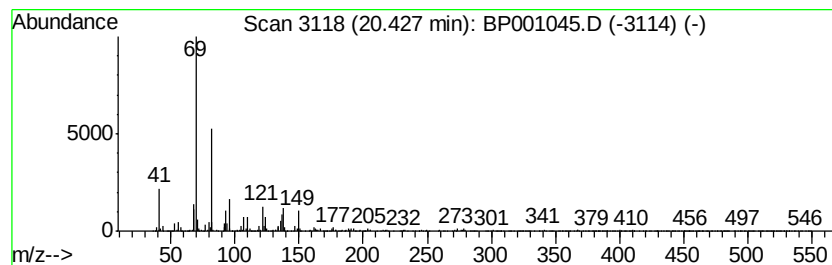
Instrument :
BNA_P
ClientSampleId :
10-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	2.12 ng	243846	Perylene-d12	21.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	99
2	Supraene	410 C30H50	007683-64-9	96
3	Docosa-2,6,10,14,18-pentaen-22-a...	384 C27H44O	1000163-04-7	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111519\
Data File : BP001045.D
Acq On : 15 Nov 2019 17:55
Operator : JU
Sample : K5832-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
10-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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
Butane, 2-methoxy...	2.33	7.8	ng	543599	1	8.36	1398520	20.0
unknown5.73	5.73	7.9	ng	551184	1	8.36	1398520	20.0
unknown8.00	8.00	53.6	ng	3748050	1	8.36	1398520	20.0
n-Hexadecanoic acid	16.53	2.2	ng	270533	4	15.65	2438000	20.0
Oxalic acid, isob...	19.17	3.2	ng	386950	5	19.29	2451780	20.0
Squalene	20.43	2.1	ng	243846	6	21.07	2302910	20.0