

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
 Data File : BG043593.D
 Acq On : 11 Nov 2019 21:16
 Operator : JU
 Sample : K5782-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-2A-COMP

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_G\METHODS\8270-BG102119.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	3.159	8	12	26	rVB	80437	153426	5.61%	1.122%
2	5.103	337	343	353	rBV	139366	224399	8.21%	1.641%
3	5.597	418	427	438	rBV	486822	863836	31.61%	6.318%
4	7.201	692	700	716	rBV	542775	1070586	39.18%	7.831%
5	7.548	751	759	771	rBV	575823	1014190	37.11%	7.418%
6	8.000	829	836	845	rBV2	97472	169838	6.21%	1.242%
7	8.323	884	891	901	rBV	438291	777760	28.46%	5.689%
8	9.163	1026	1034	1050	rBV	294878	608347	22.26%	4.450%
9	10.808	1303	1314	1324	rBV	100815	216659	7.93%	1.585%
10	13.253	1722	1730	1744	rBV	969815	1621129	59.32%	11.858%
11	14.087	1866	1872	1883	rBV2	34473	75369	2.76%	0.551%
12	14.633	1958	1965	1976	rBV	206042	367541	13.45%	2.688%
13	16.126	2212	2219	2239	rBV	832088	1475065	53.98%	10.789%
14	17.377	2425	2432	2448	rBV	270115	495606	18.14%	3.625%
15	18.270	2579	2584	2588	rBV3	28786	44892	1.64%	0.328%
16	19.986	2870	2876	2892	rBV	2007201	2732763	100.00%	19.989%
17	21.290	3092	3098	3109	rBV5	39794	132349	4.84%	0.968%
18	21.367	3109	3111	3121	rVB6	14609	32055	1.17%	0.234%
19	21.643	3151	3158	3172	rBV2	282300	529190	19.36%	3.871%
20	21.825	3184	3189	3194	rVB	23483	35235	1.29%	0.258%
21	22.418	3286	3290	3298	rBV3	26197	41789	1.53%	0.306%
22	23.088	3397	3404	3414	rBV4	72150	171591	6.28%	1.255%
23	23.294	3433	3439	3450	rVB	94102	176663	6.46%	1.292%
24	23.899	3535	3542	3548	rVB3	25983	52399	1.92%	0.383%
25	24.827	3690	3700	3713	rVB2	196349	588912	21.55%	4.308%

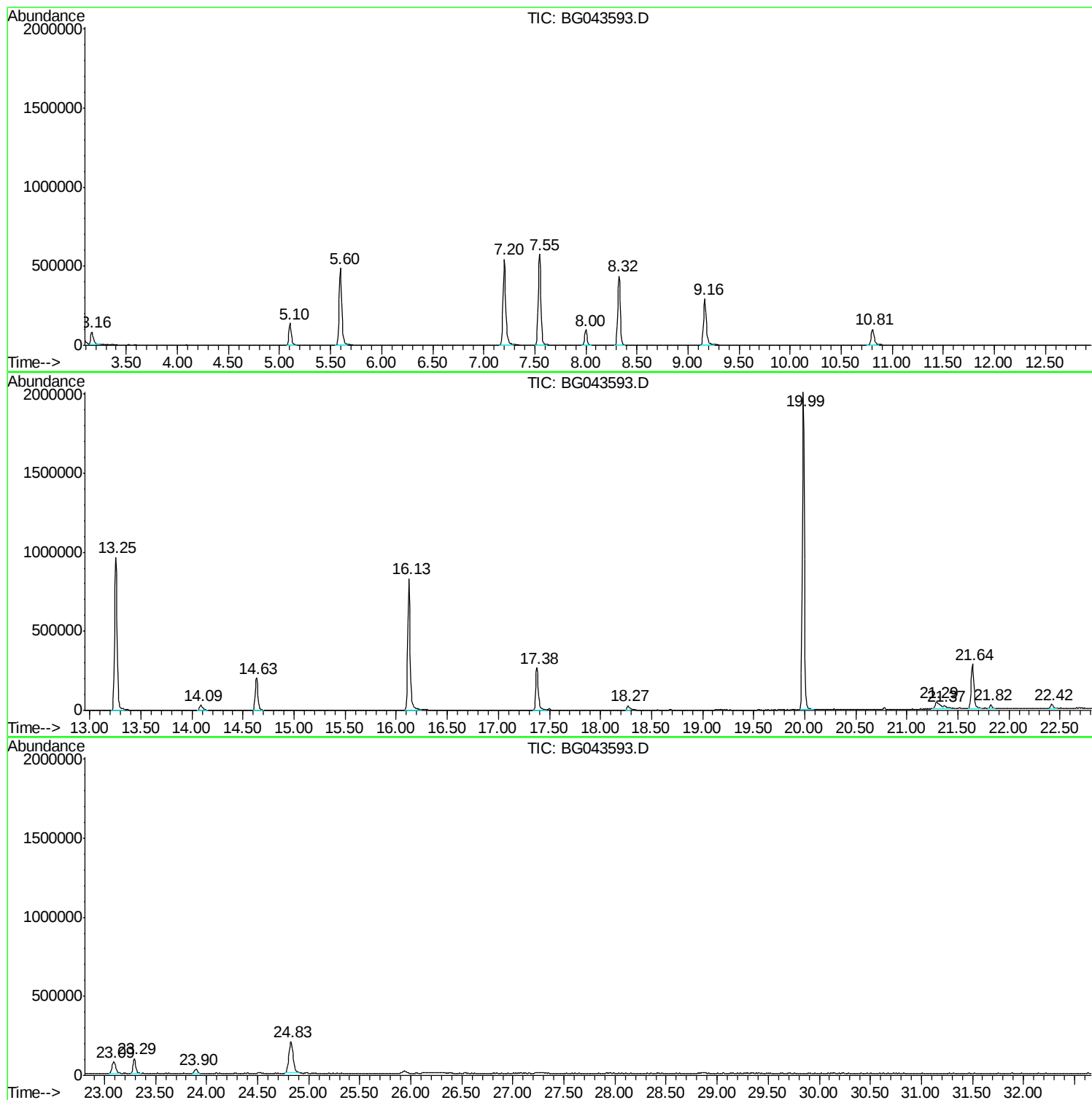
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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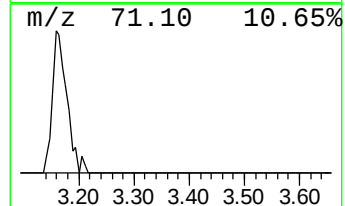
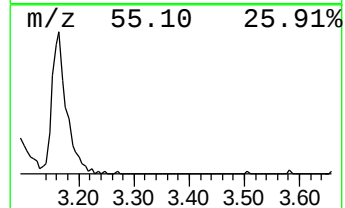
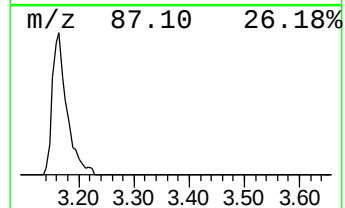
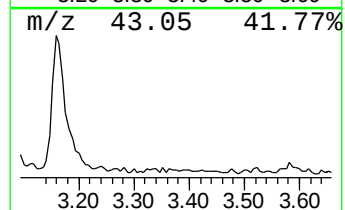
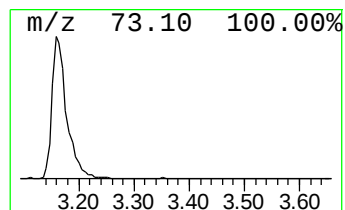
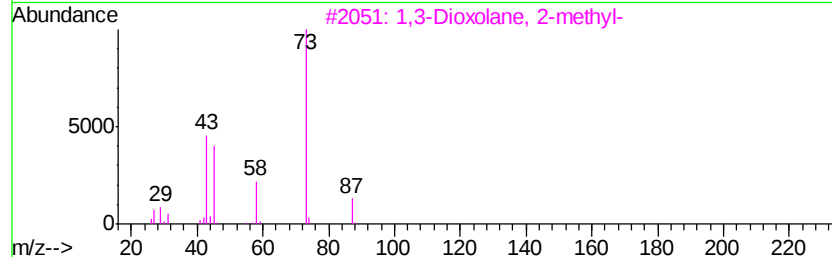
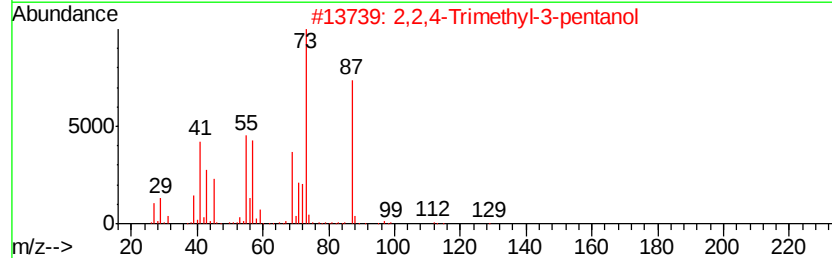
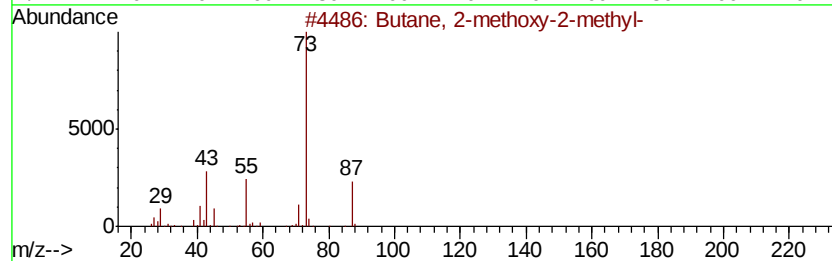
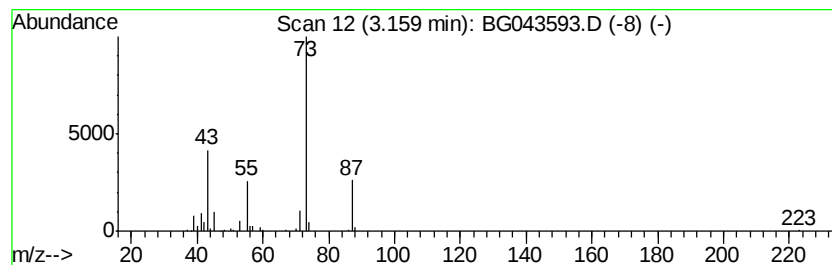
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	18.07 ng	153426	1,4-Dichlorobenzene-d4	8.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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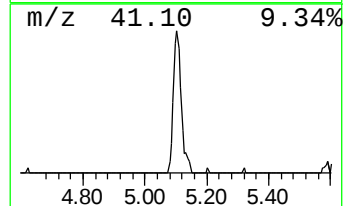
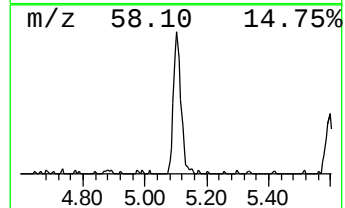
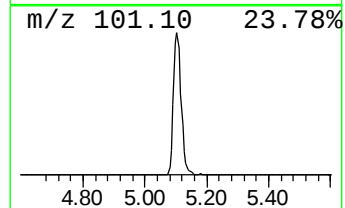
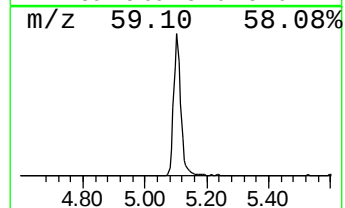
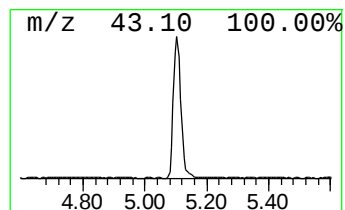
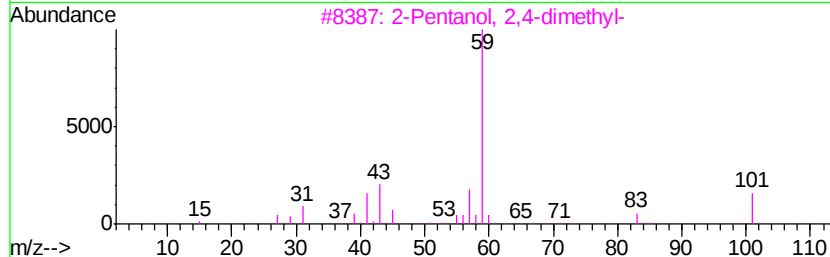
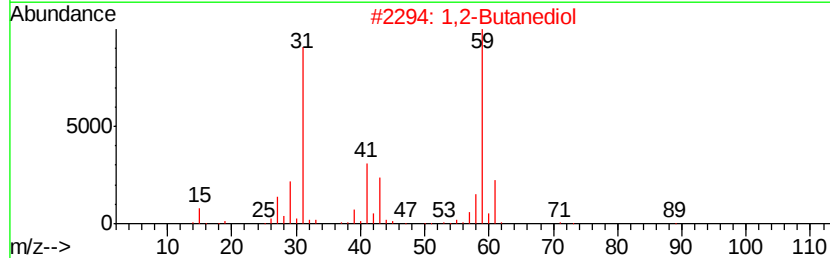
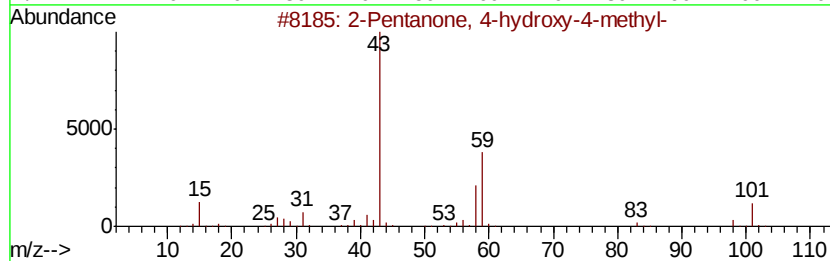
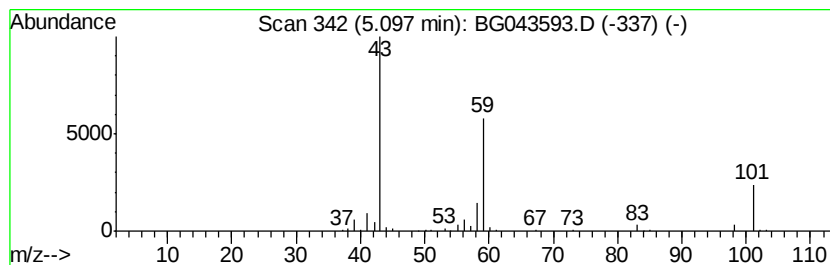
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	26.43 ng	224399	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,2-Butanediol	90	C4H10O2	000584-03-2	32
3		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4		Guanidine	59	CH5N3	000113-00-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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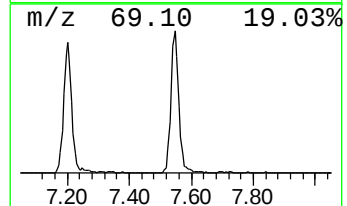
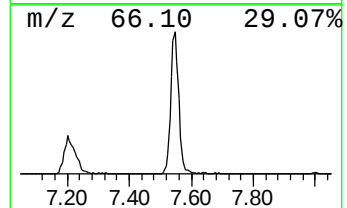
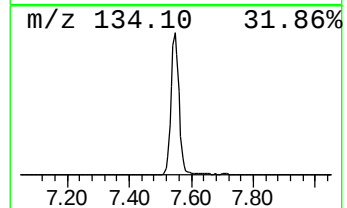
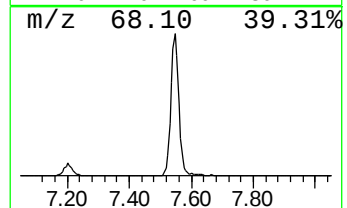
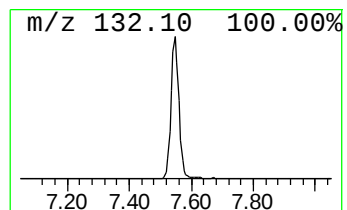
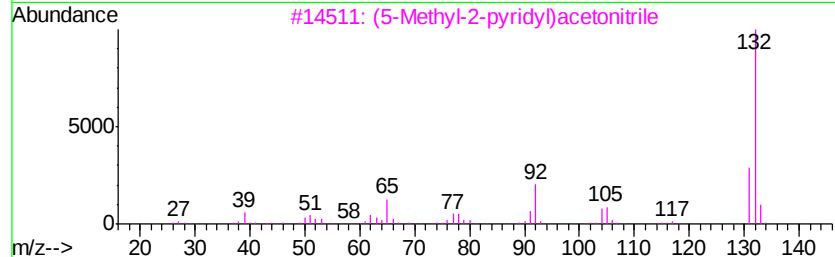
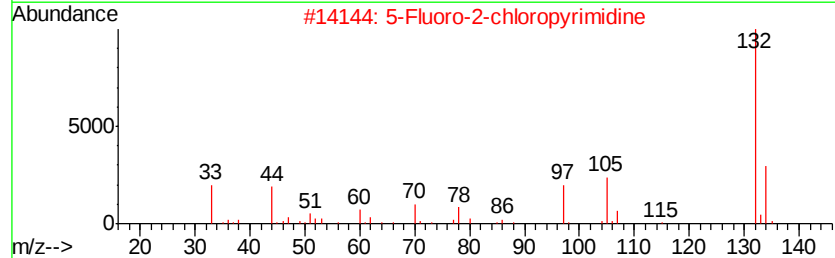
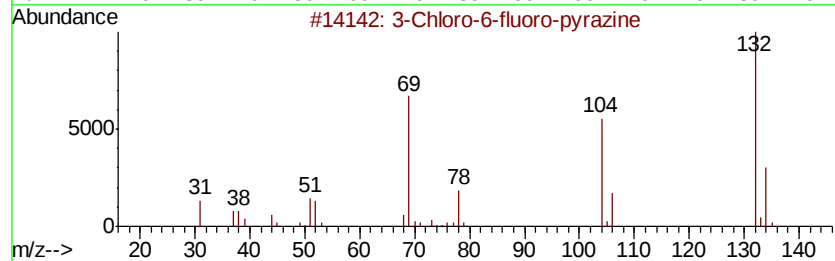
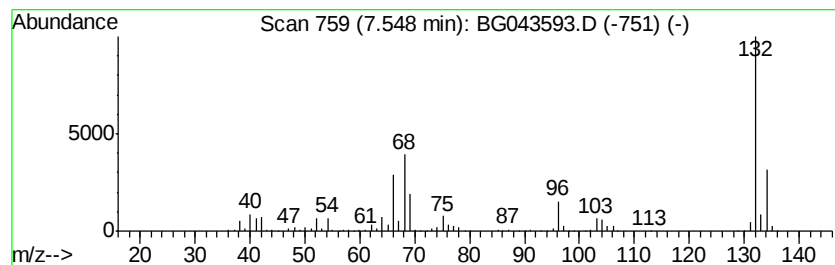
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Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	119.43 ng	1014190	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12	
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10	
5	N-(3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10	



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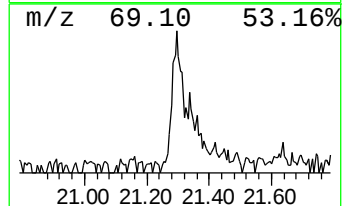
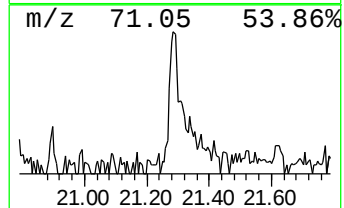
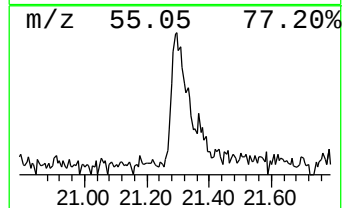
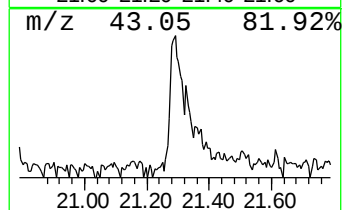
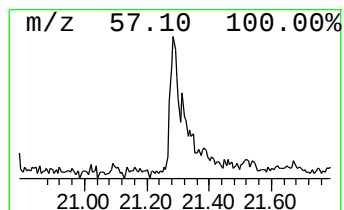
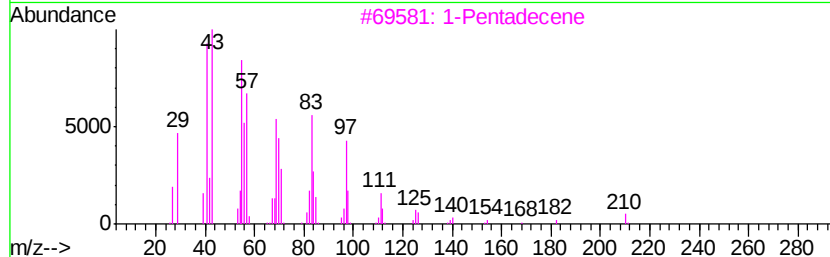
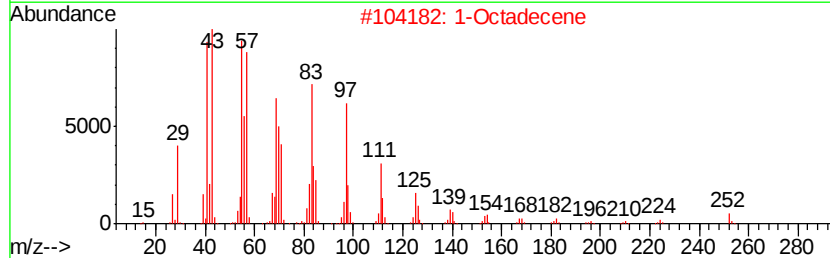
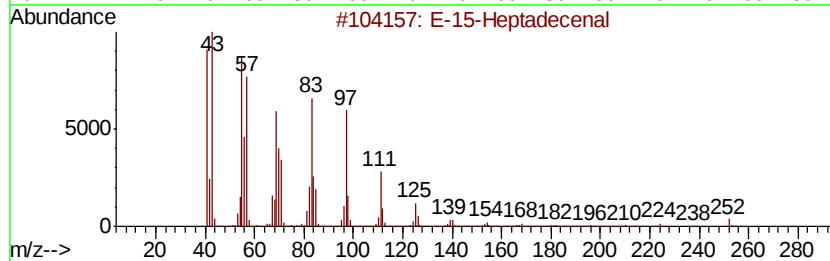
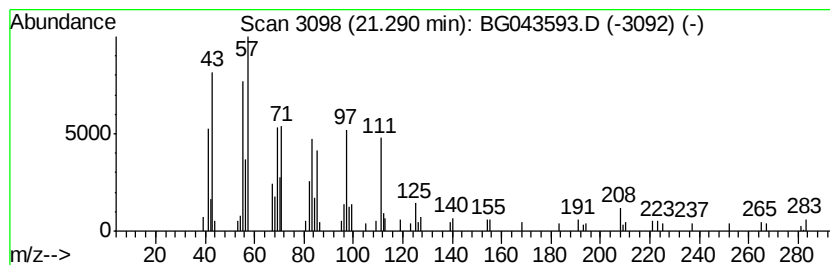
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Peak Number 5 E-15-Heptadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.29	5.00 ng	132349	Chrysene-d12	21.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	1-Octadecene	252	C18H36	000112-88-9	86
3	1-Pentadecene	210	C15H30	013360-61-7	83
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70



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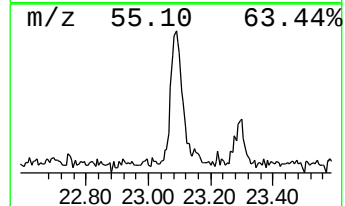
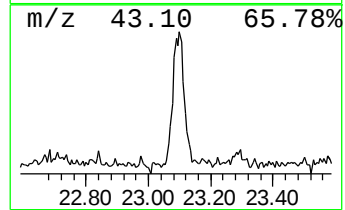
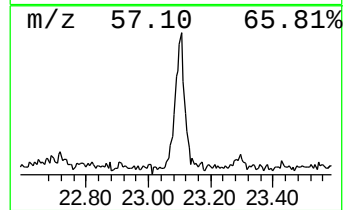
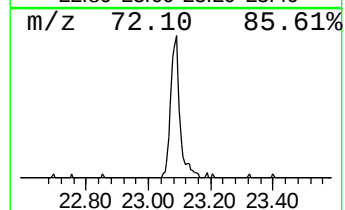
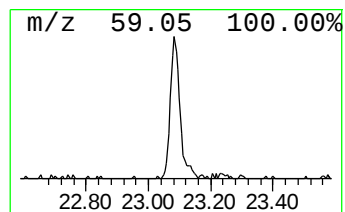
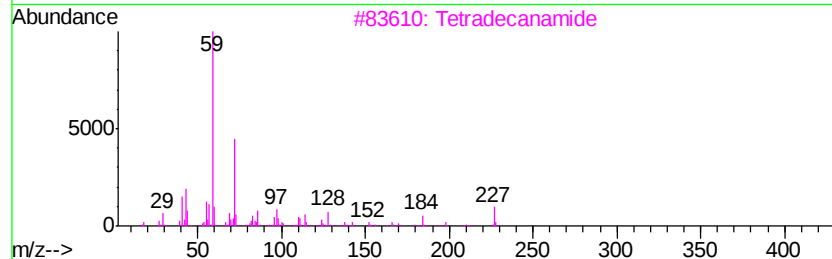
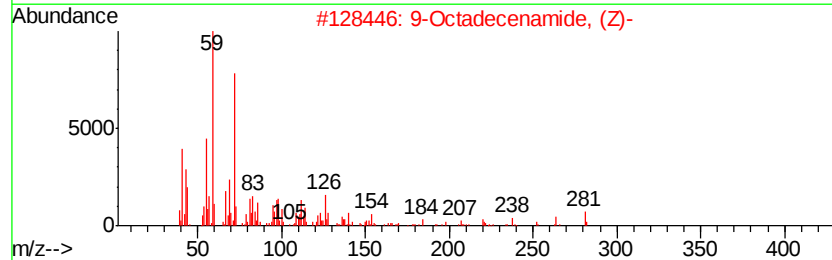
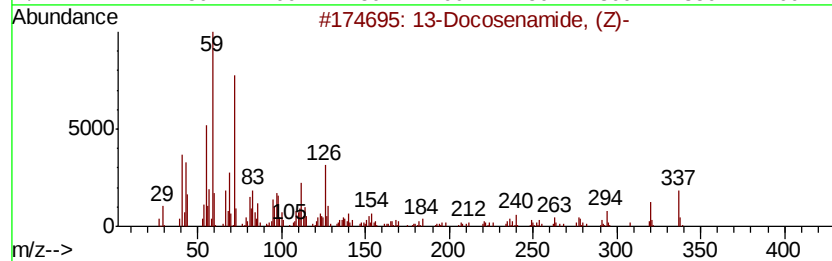
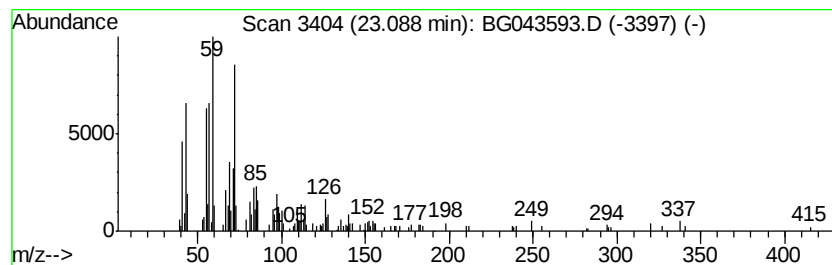
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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	6.49 ng	171591	Chrysene-d12	21.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	38
5		3-Tetradecanone	212	C14H28O	000629-23-2	38



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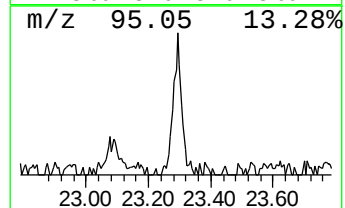
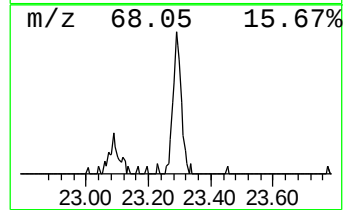
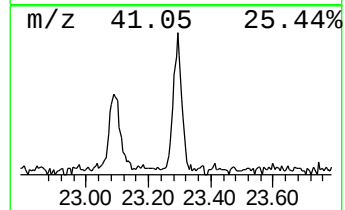
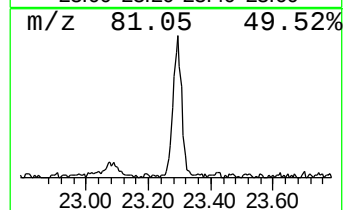
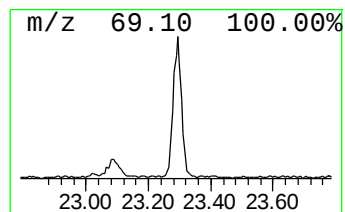
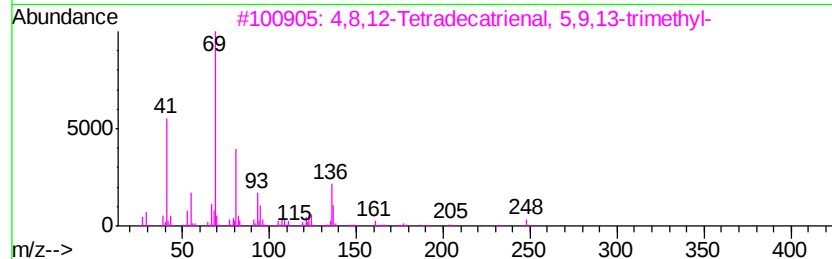
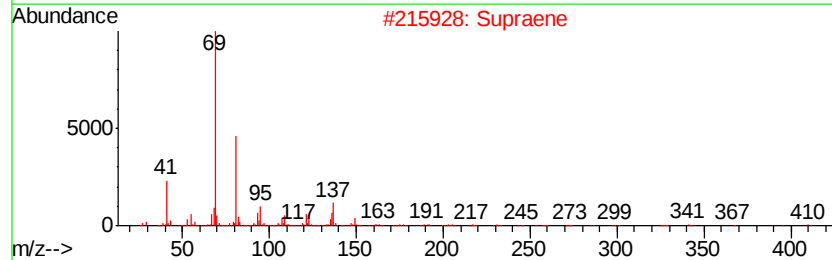
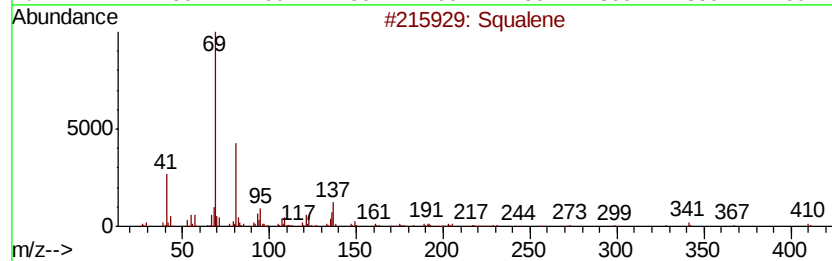
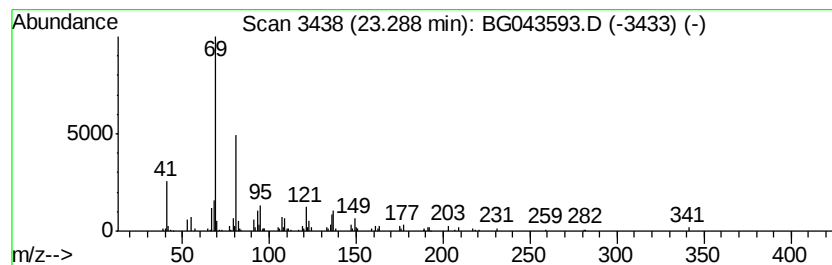
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	6.00 ng	176663	Perylene-d12	24.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	86
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111119\
Data File : BG043593.D
Acq On : 11 Nov 2019 21:16
Operator : JU
Sample : K5782-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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...	3.16	18.1	ng	153426	1	8.00	169838	20.0
2-Pentanone, 4-hy...	5.10	26.4	ng	224399	1	8.00	169838	20.0
unknown7.55	7.55	119.4	ng	1014190	1	8.00	169838	20.0
E-15-Heptadecenal	21.29	5.0	ng	132349	5	21.64	529190	20.0
13-Docosenamide, ...	23.09	6.5	ng	171591	5	21.64	529190	20.0
Squalene	23.29	6.0	ng	176663	6	24.83	588912	20.0