

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131675.D
 Acq On : 16 Dec 2022 19:50
 Operator : CG\JU
 Sample : N6037-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-23-(0.5-2.5)

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	19	rVB	330612	406848	19.51%	2.995%
2	4.457	399	403	411	rBV	63026	72087	3.46%	0.531%
3	5.087	505	510	520	rVB	411824	488046	23.40%	3.593%
4	5.493	575	579	582	rBV	1519049	1337605	64.13%	9.847%
5	6.510	747	752	755	rBV	1681119	1608918	77.14%	11.844%
6	6.881	811	815	818	rBV	514351	415098	19.90%	3.056%
7	7.445	906	911	914	rBV	1206512	1084040	51.97%	7.980%
8	8.169	1030	1034	1037	rBV	640568	517431	24.81%	3.809%
9	9.251	1212	1218	1221	rBV	2304654	1996238	95.70%	14.695%
10	9.933	1330	1334	1337	rBV	659364	595248	28.54%	4.382%
11	10.645	1452	1455	1459	rBV	154910	134326	6.44%	0.989%
12	10.722	1464	1468	1479	rBV	880603	735908	35.28%	5.417%
13	11.427	1584	1588	1590	rBV	761890	634050	30.40%	4.667%
14	11.451	1590	1592	1595	rVB	60244	48270	2.31%	0.355%
15	12.645	1792	1795	1798	rBV	75852	59720	2.86%	0.440%
16	12.874	1828	1834	1838	rVB	67937	66841	3.20%	0.492%
17	13.021	1854	1859	1862	rBV	2506529	2085844	100.00%	15.355%
18	13.921	2008	2012	2032	rBV4	47340	160395	7.69%	1.181%
19	14.080	2032	2039	2042	rBV	500227	462016	22.15%	3.401%
20	14.174	2051	2055	2060	rVB2	28300	32167	1.54%	0.237%
21	14.939	2181	2185	2189	rBV	52768	50160	2.40%	0.369%
22	15.210	2227	2231	2236	rVB	24486	26656	1.28%	0.196%
23	15.580	2289	2294	2304	rBV	295530	410475	19.68%	3.022%
24	16.057	2370	2375	2383	rVB2	23982	38588	1.85%	0.284%
25	16.586	2459	2465	2471	rBV3	19814	32480	1.56%	0.239%
26	17.098	2544	2552	2559	rBV3	9357	25231	1.21%	0.186%
27	17.209	2564	2571	2576	rVB5	13678	29753	1.43%	0.219%
28	17.939	2686	2695	2701	rBV8	11191	30100	1.44%	0.222%

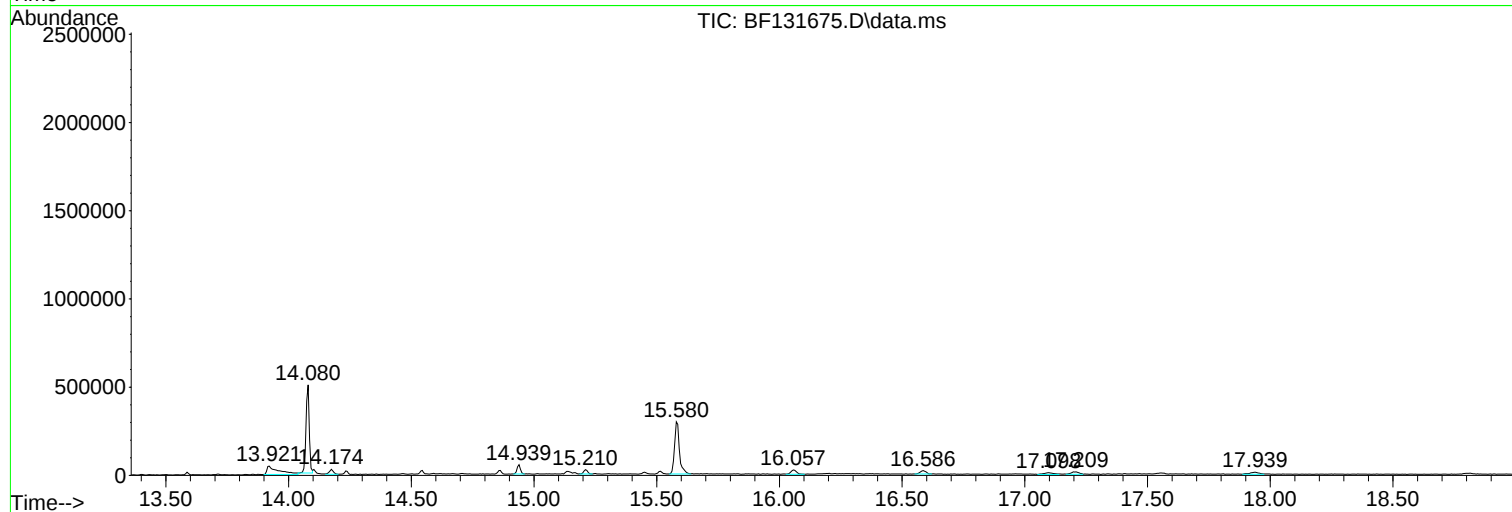
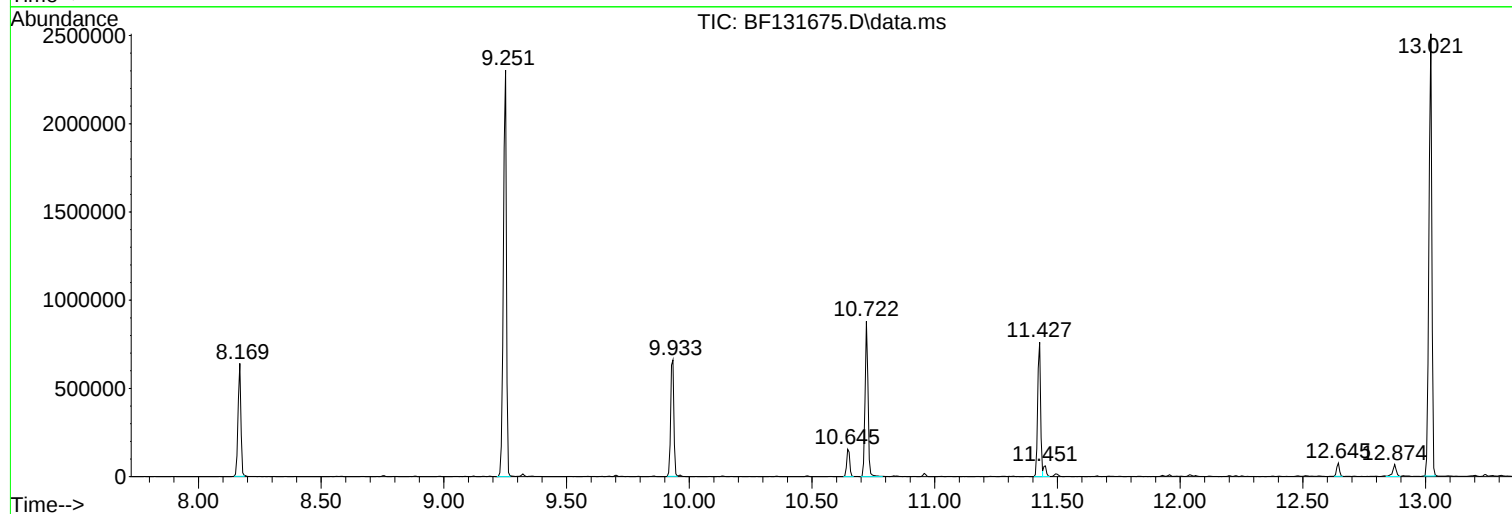
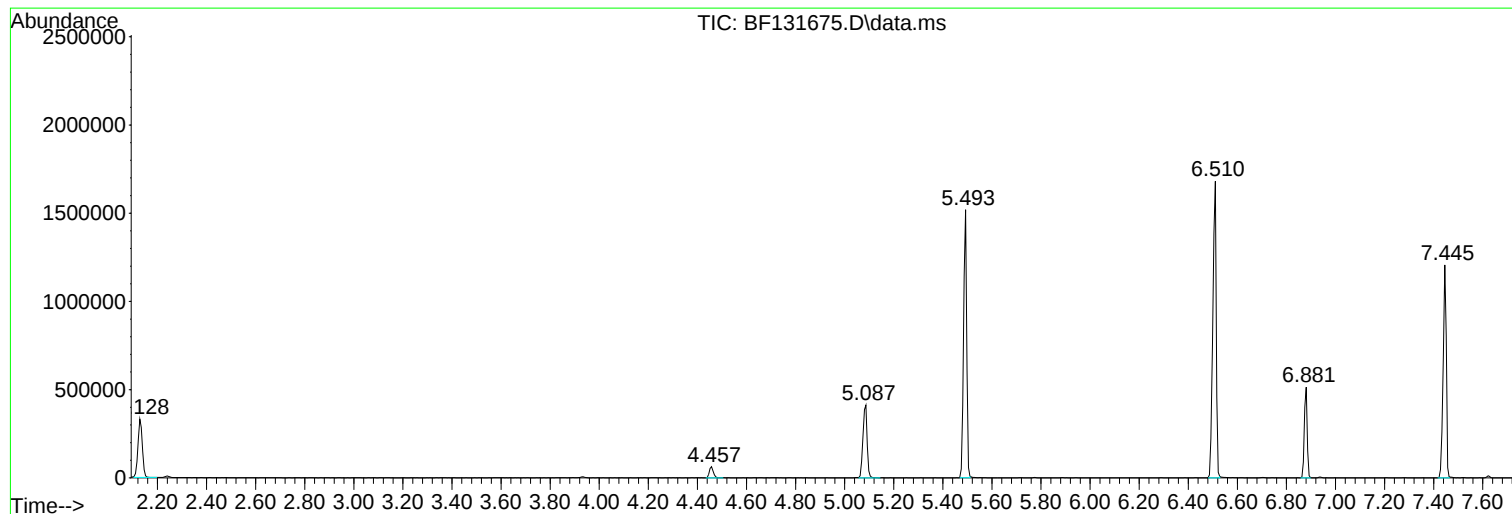
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ClientSampleId :
RB-23-(0.5-2.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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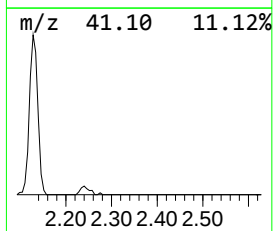
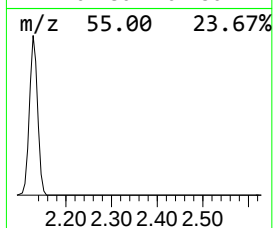
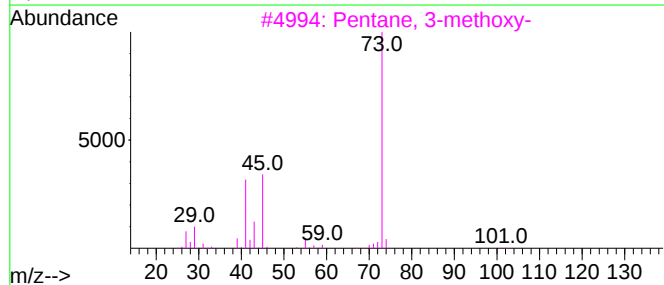
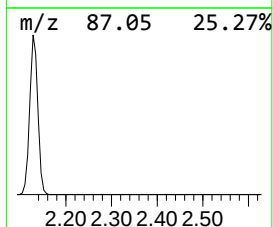
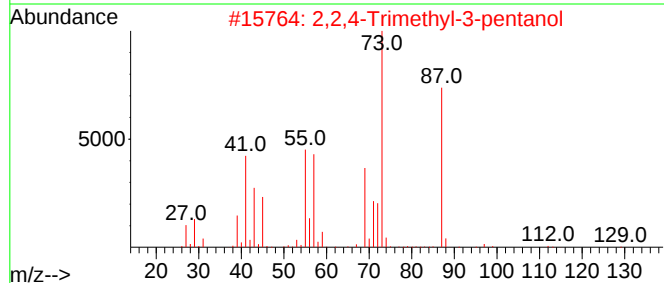
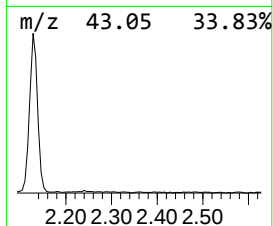
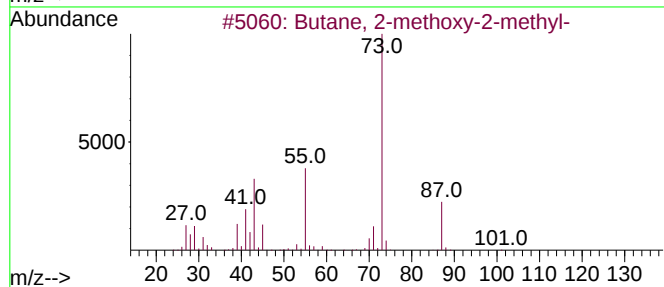
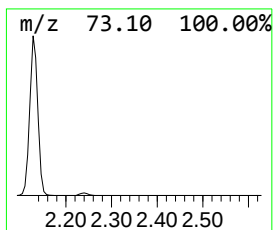
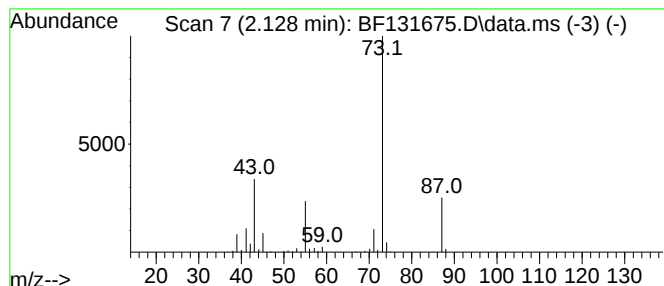
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	19.60 ng	406848	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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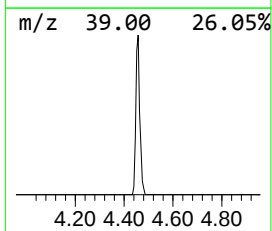
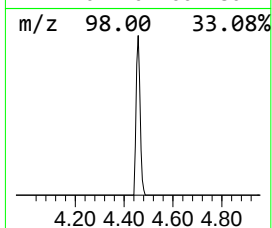
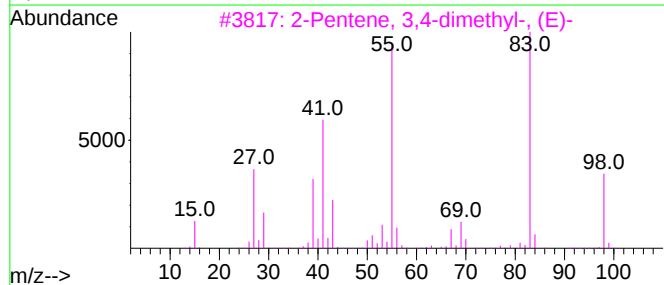
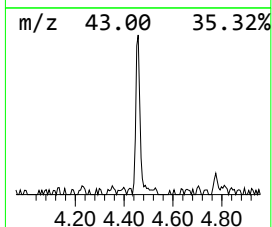
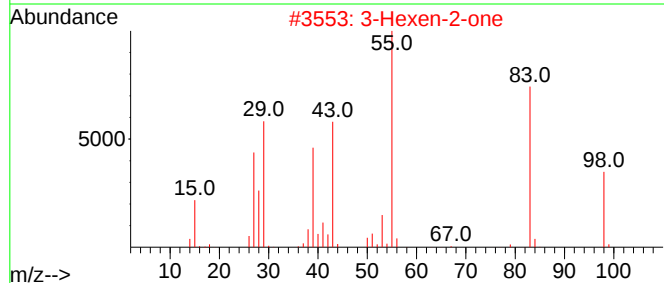
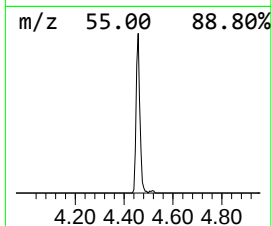
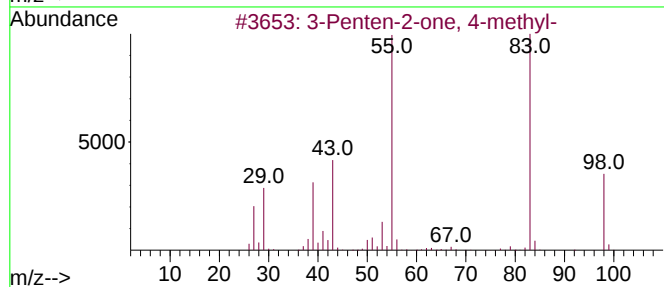
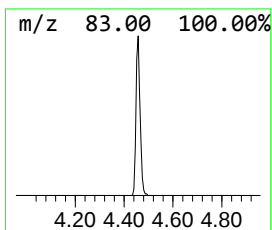
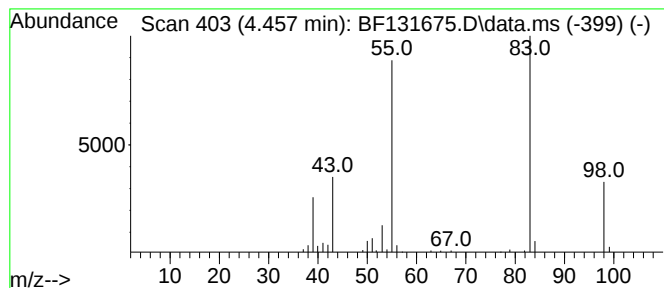
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	3.47 ng	72087	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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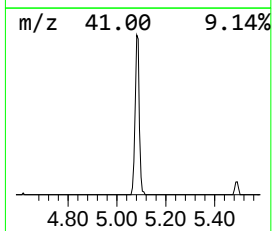
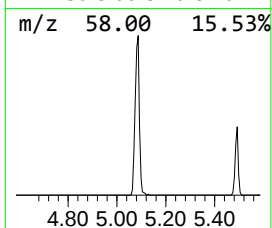
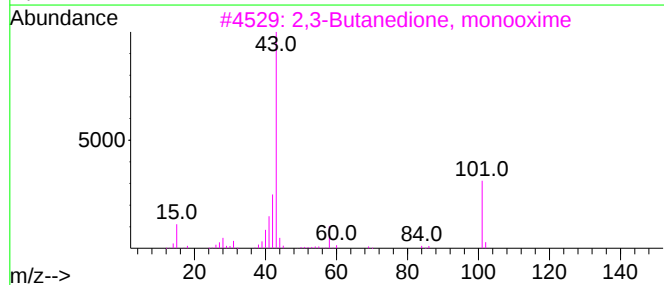
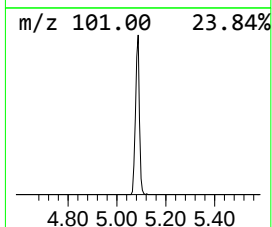
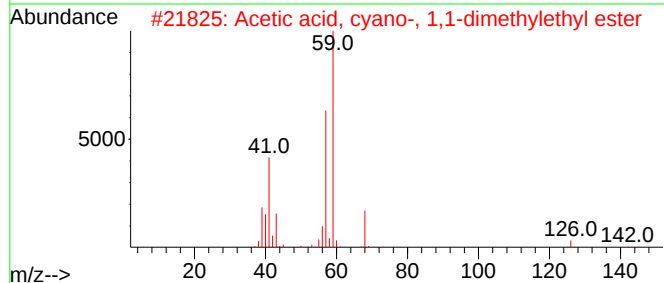
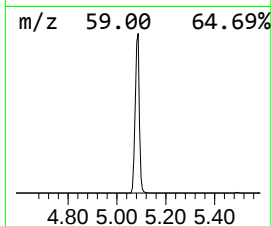
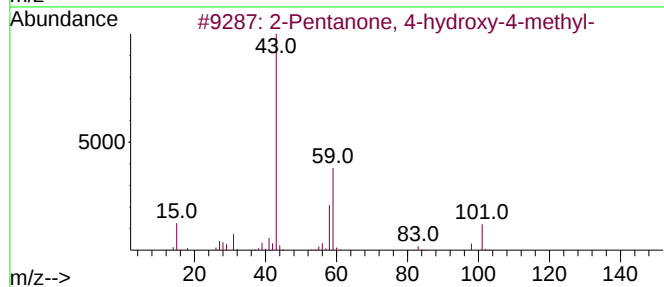
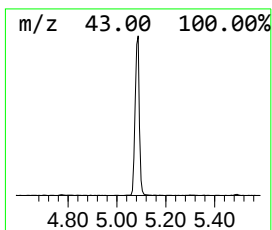
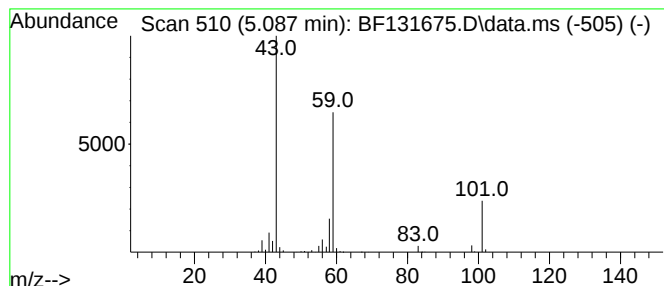
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	23.51 ng	488046	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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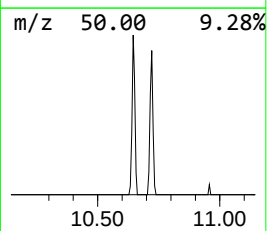
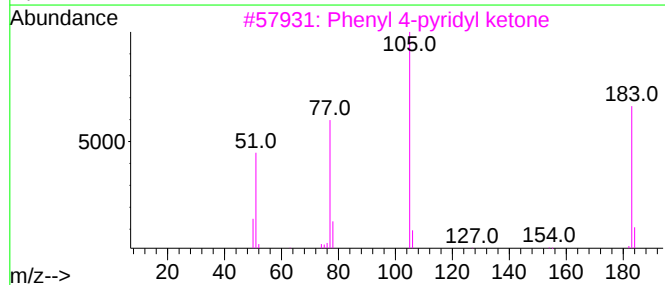
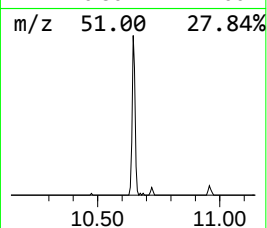
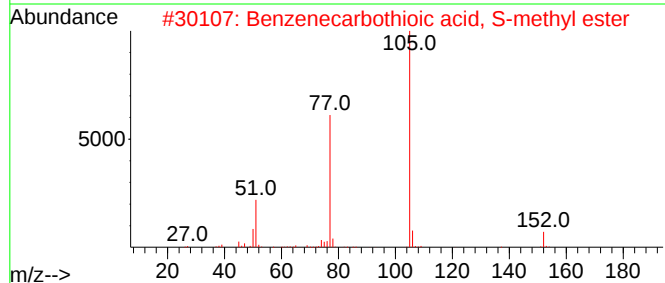
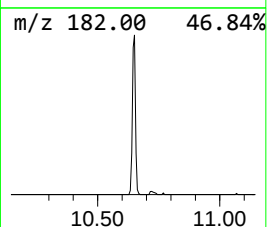
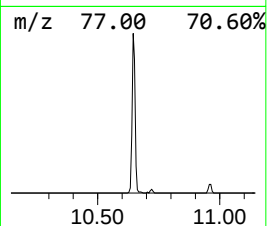
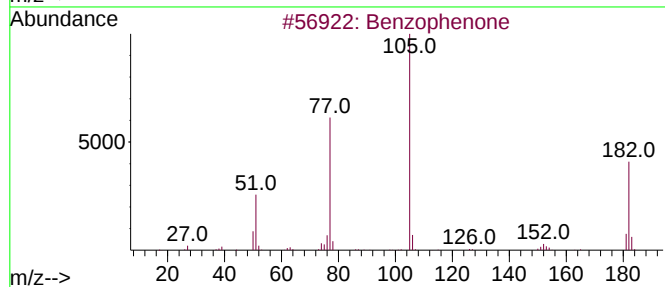
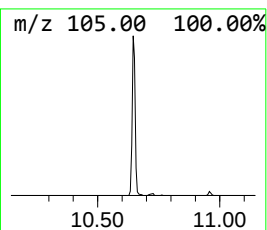
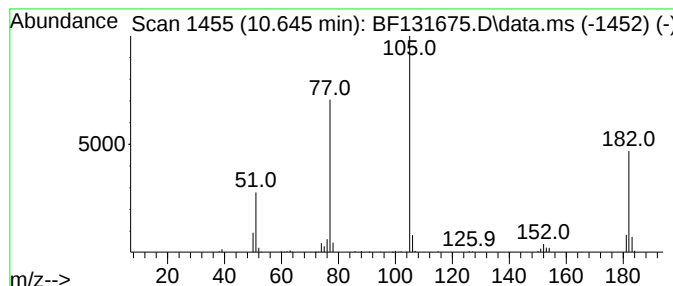
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	4.51 ng	134326	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
4			N-cyanobenzamide	146	C8H6N2O	015150-25-1	49
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



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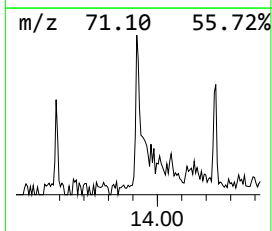
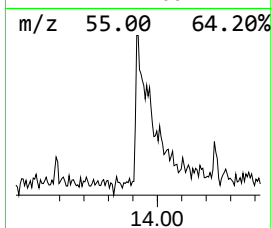
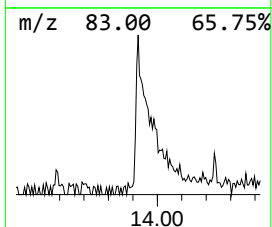
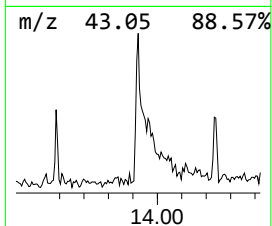
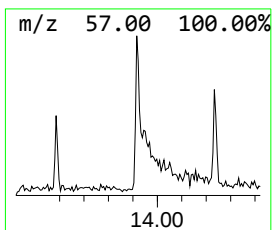
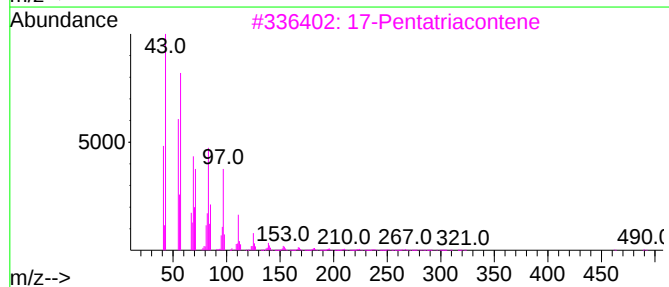
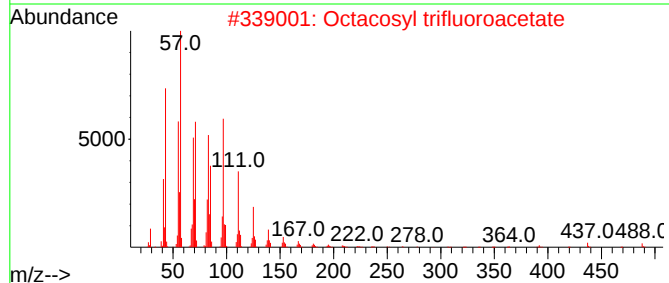
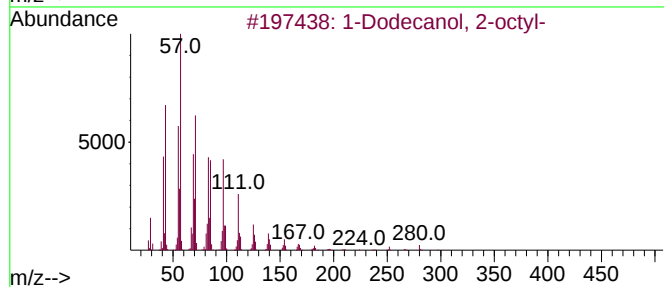
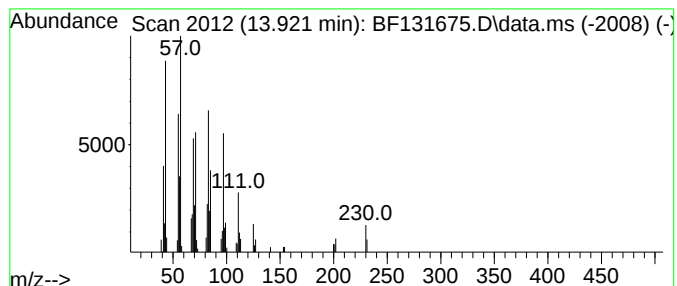
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	6.94 ng	160395	Chrysene-d12	14.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
3		17-Pentatriacontene	491	C35H70	006971-40-0	87
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83



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RB-23-(0.5-2.5)

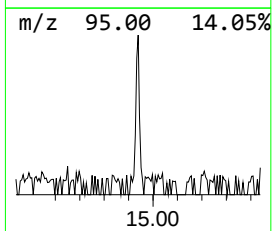
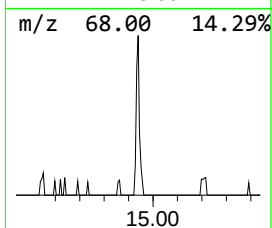
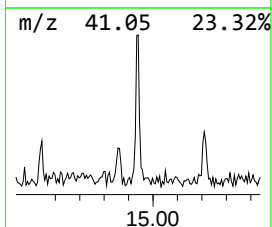
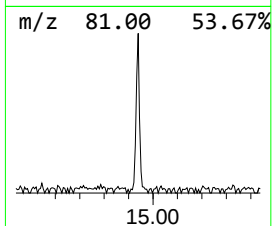
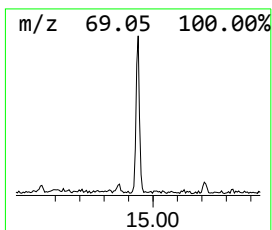
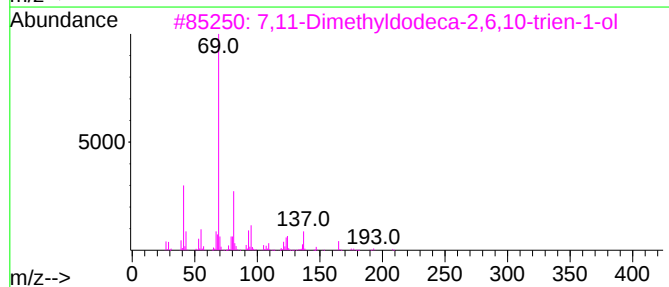
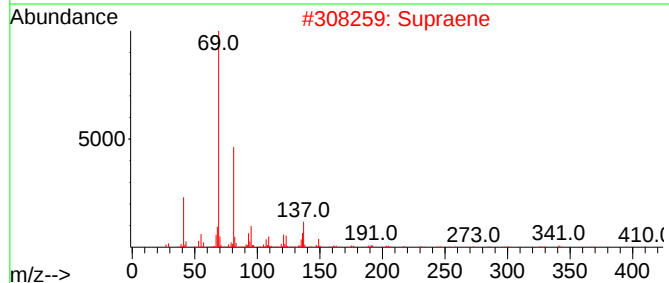
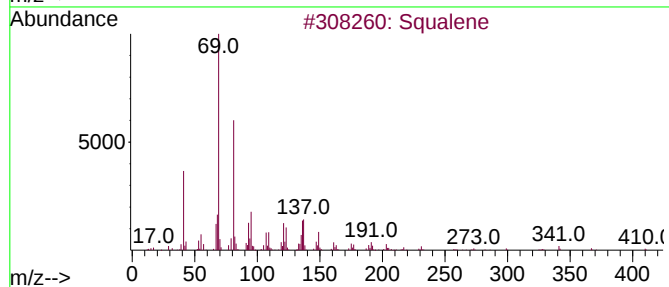
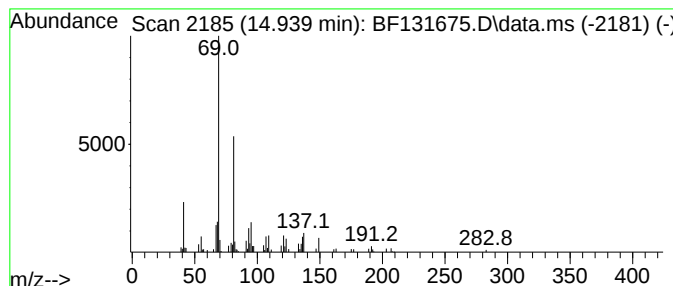
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.44 ng	50160	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	83
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4			trans-Farnesol	222	C15H26O	000106-28-5	78
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131675.D
Acq On : 16 Dec 2022 19:50
Operator : CG\JU
Sample : N6037-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-23-(0.5-2.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	19.6	ng	406848	1	6.881	415098	20.0
3-Penten-2-one,...	4.457	3.5	ng	72087	1	6.881	415098	20.0
2-Pentanone, 4-...	5.087	23.5	ng	488046	1	6.881	415098	20.0
Benzophenone	10.645	4.5	ng	134326	3	9.933	595248	20.0
1-Dodecanol, 2-...	13.921	6.9	ng	160395	5	14.080	462016	20.0
Squalene	14.939	2.4	ng	50160	6	15.580	410475	20.0