

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131678.D
 Acq On : 16 Dec 2022 21:28
 Operator : CG\JU
 Sample : N6037-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-26-(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

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

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	449258	539867	27.44%	3.937%
2	4.457	399	403	413	rBV	178250	192740	9.79%	1.405%
3	5.081	505	509	518	rVB	403721	455417	23.14%	3.321%
4	5.492	575	579	582	rBV	1199141	1038236	52.76%	7.571%
5	6.510	747	752	755	rBV	1712111	1624110	82.53%	11.843%
6	6.881	811	815	818	rBV	554708	460965	23.43%	3.361%
7	7.445	906	911	914	rBV	1225299	1088202	55.30%	7.935%
8	8.169	1030	1034	1037	rBV	710948	578393	29.39%	4.218%
9	9.251	1213	1218	1221	rBV	2143853	1967797	100.00%	14.349%
10	9.933	1330	1334	1337	rBV	767677	663948	33.74%	4.842%
11	10.645	1452	1455	1459	rBV	111804	93383	4.75%	0.681%
12	10.722	1464	1468	1477	rBV	657223	527772	26.82%	3.849%
13	10.833	1484	1487	1494	rVB	30410	27066	1.38%	0.197%
14	10.957	1505	1508	1511	rBV	28806	22754	1.16%	0.166%
15	11.427	1584	1588	1590	rBV	873039	705258	35.84%	5.143%
16	11.451	1590	1592	1595	rVB	41309	30354	1.54%	0.221%
17	11.951	1675	1677	1681	rVB2	25586	24755	1.26%	0.181%
18	12.645	1791	1795	1799	rVB	93143	82684	4.20%	0.603%
19	12.874	1829	1834	1838	rBV	113315	111629	5.67%	0.814%
20	13.021	1854	1859	1862	rBV	2308204	1960457	99.63%	14.296%
21	13.586	1951	1955	1958	rBV2	22457	22539	1.15%	0.164%
22	13.921	2008	2012	2022	rBV7	41739	115012	5.84%	0.839%
23	14.080	2032	2039	2042	rBV	524472	524806	26.67%	3.827%
24	14.104	2042	2043	2050	rVB	39491	25105	1.28%	0.183%
25	14.174	2050	2055	2060	rVB	32126	36569	1.86%	0.267%
26	14.545	2114	2118	2122	rBV3	22395	25469	1.29%	0.186%
27	14.857	2168	2171	2175	rBV2	22280	22292	1.13%	0.163%
28	14.939	2180	2185	2189	rBV	47022	52145	2.65%	0.380%
29	15.139	2212	2219	2222	rBV3	25268	43999	2.24%	0.321%
30	15.209	2227	2231	2235	rVB	25695	27794	1.41%	0.203%
31	15.515	2278	2283	2288	rBV	26760	34314	1.74%	0.250%
32	15.580	2289	2294	2306	rVB	340975	451891	22.96%	3.295%
33	16.056	2368	2375	2380	rBV2	26569	42054	2.14%	0.307%
34	16.586	2459	2465	2472	rBV3	19679	37755	1.92%	0.275%
35	17.203	2564	2570	2577	rVB5	14586	31752	1.61%	0.232%
36	17.545	2624	2628	2637	rBV3	9834	24214	1.23%	0.177%

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RB-26-(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

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

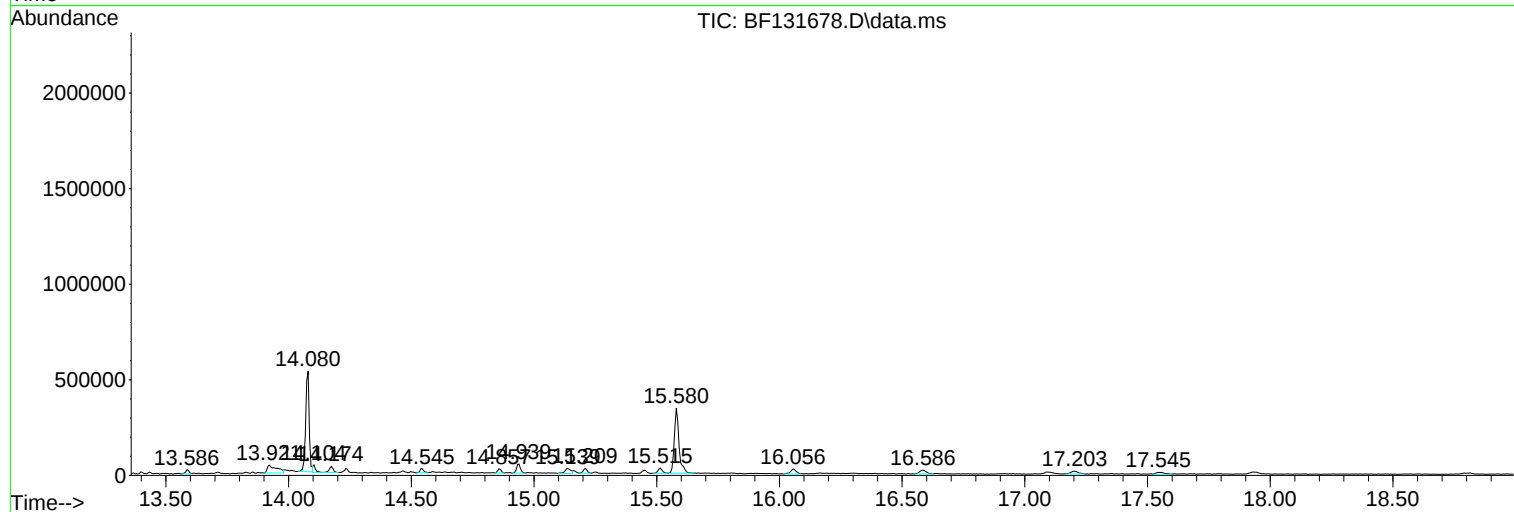
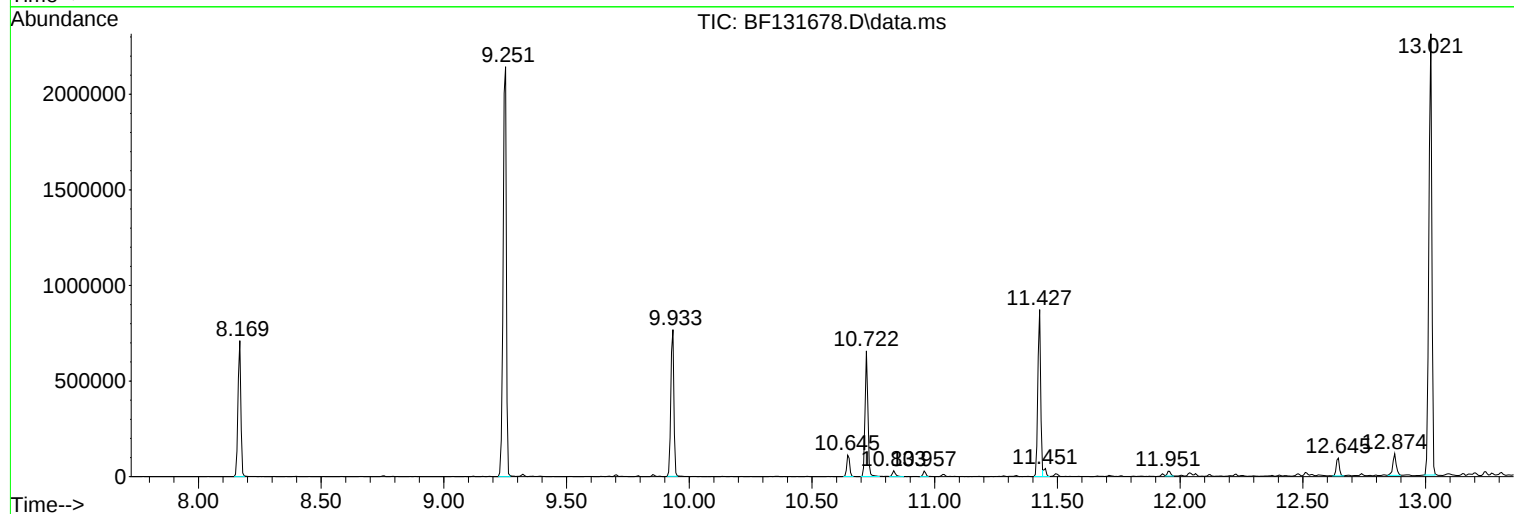
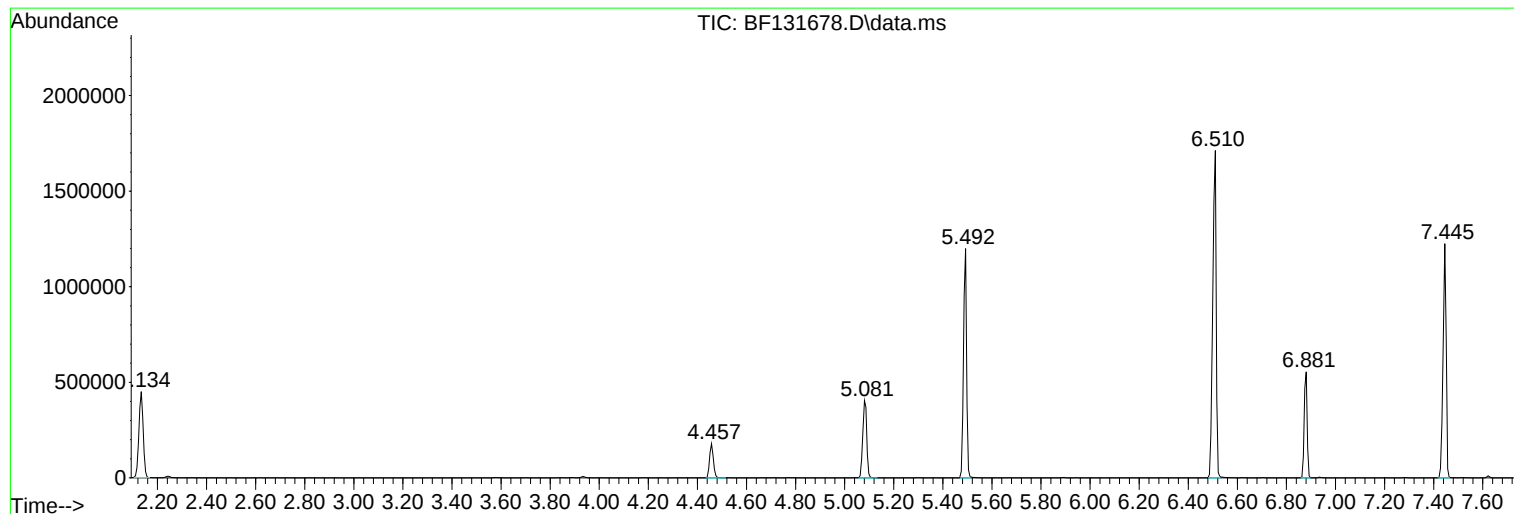
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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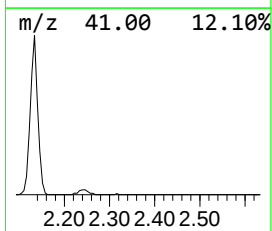
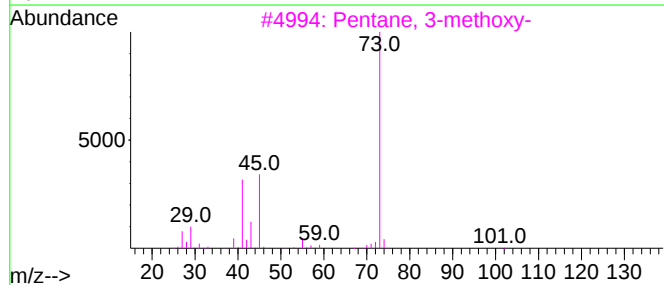
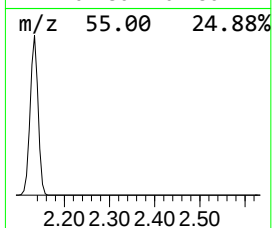
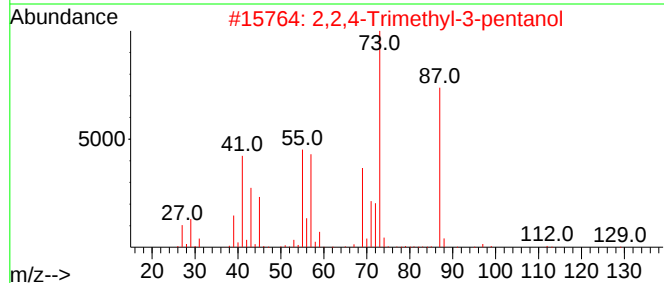
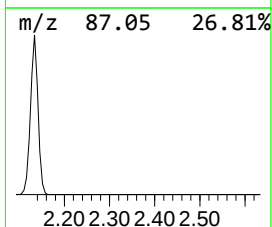
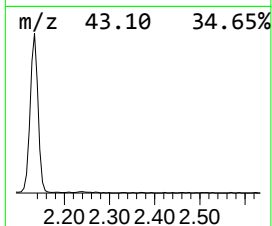
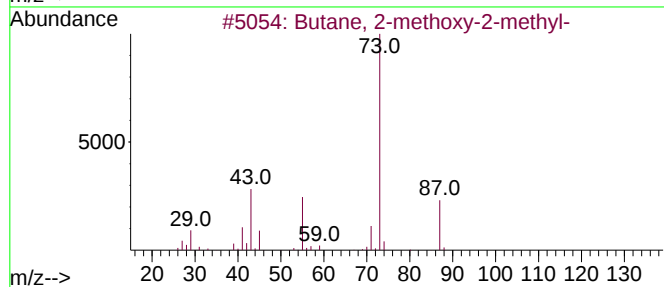
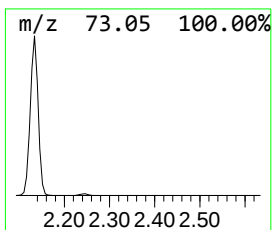
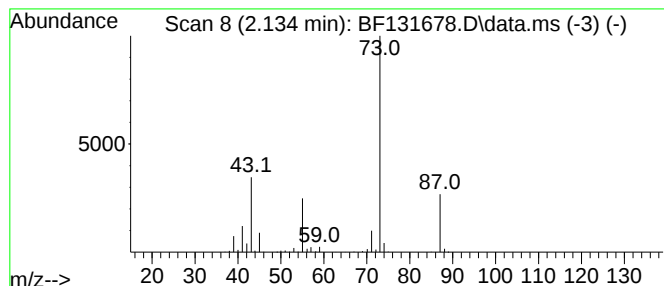
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	23.42 ng	539867	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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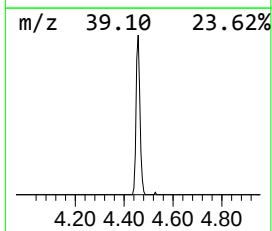
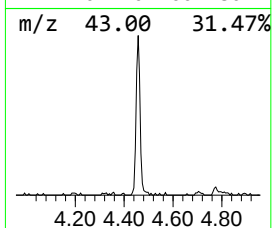
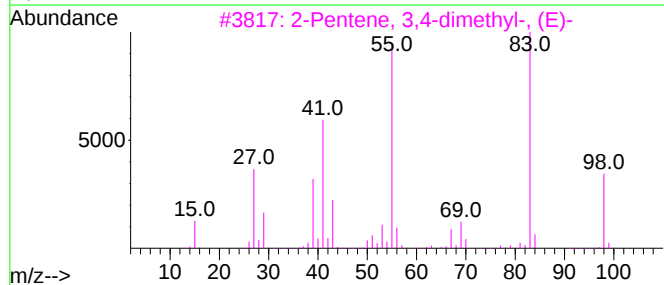
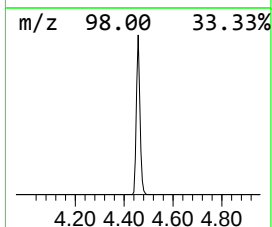
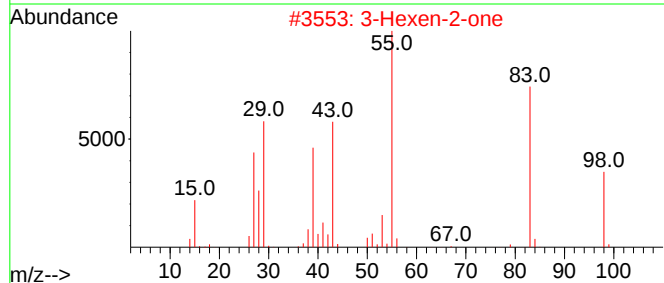
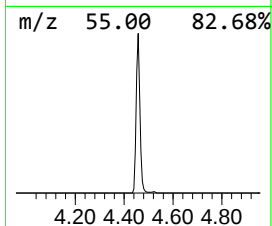
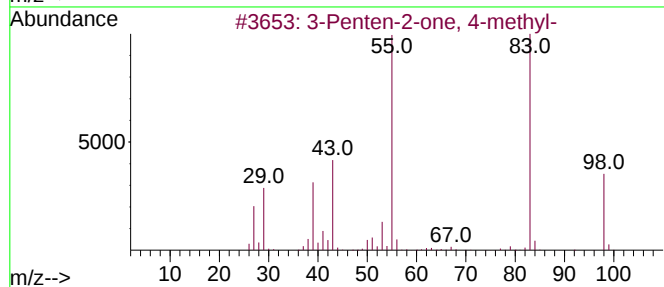
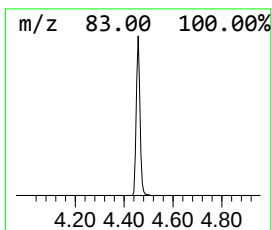
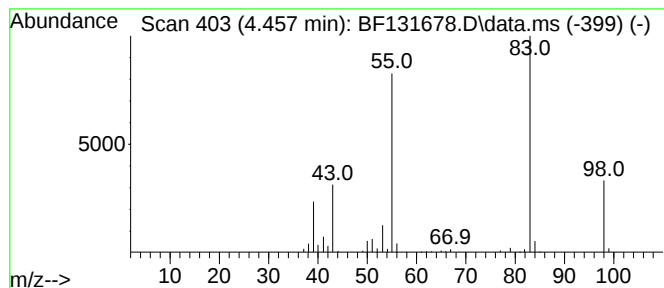
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	8.36 ng	192740	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	80
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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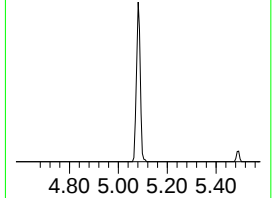
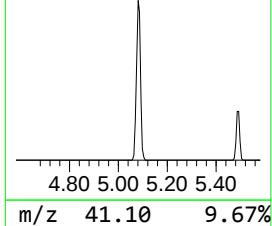
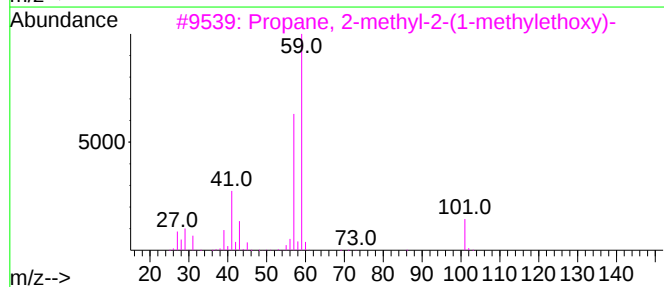
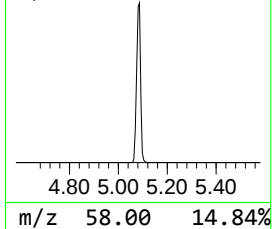
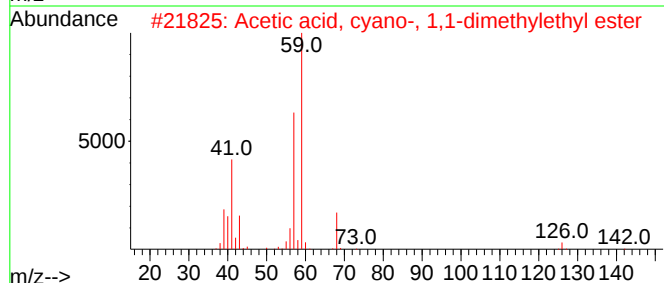
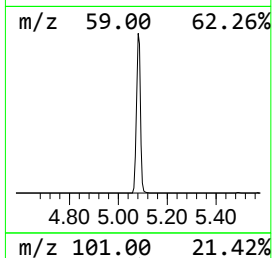
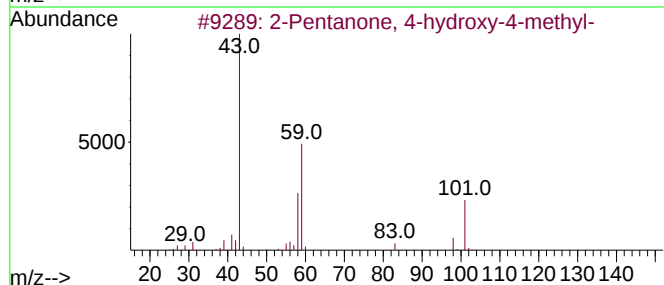
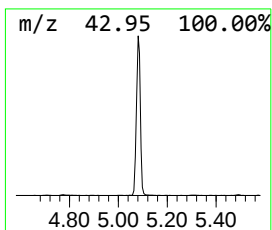
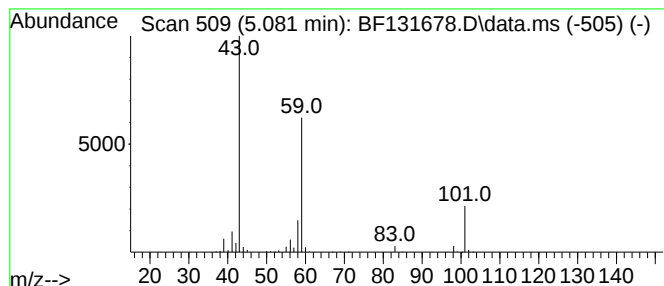
Instrument :
BNA_F
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RB-26-(2-4)

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.081	19.76 ng	455417	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	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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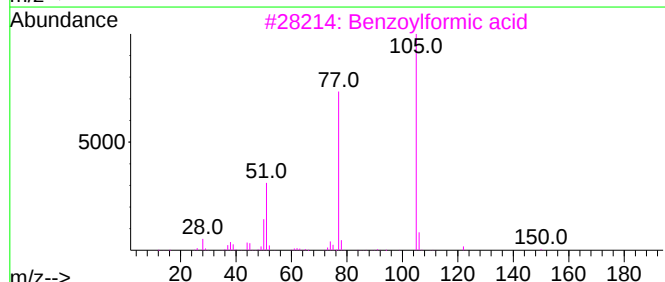
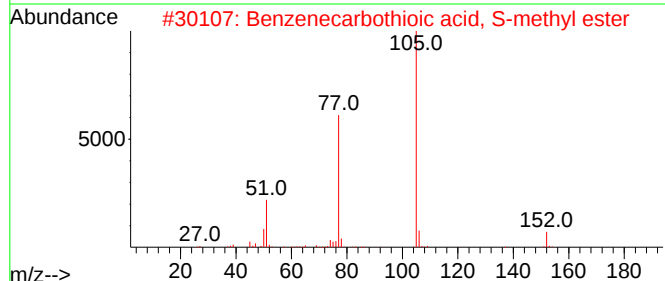
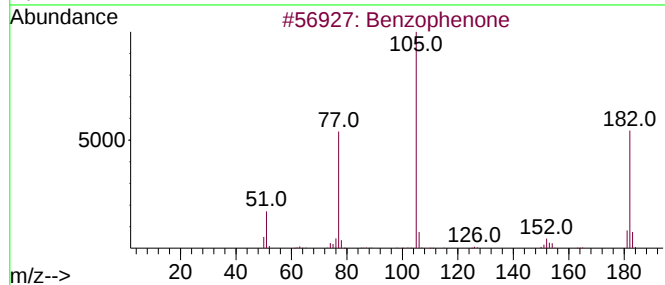
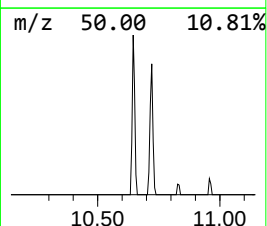
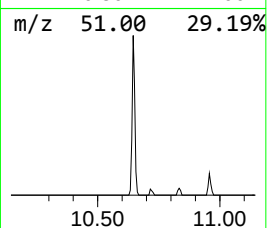
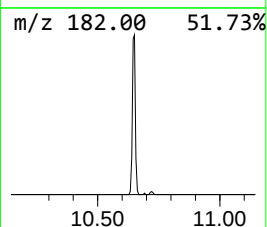
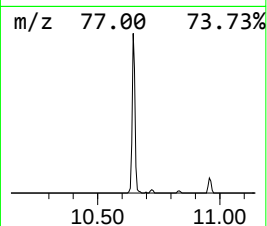
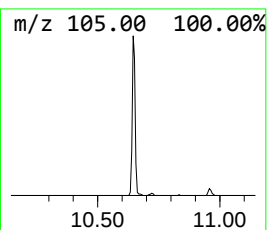
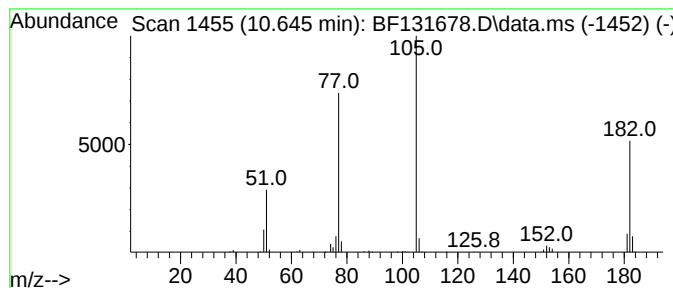
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	2.81 ng	93383	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	62
3			Benzoylformic acid	150	C8H6O3	000611-73-4	58
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	53
5			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	53



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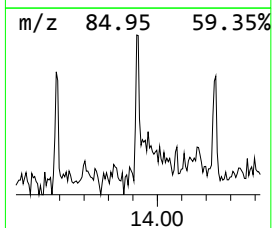
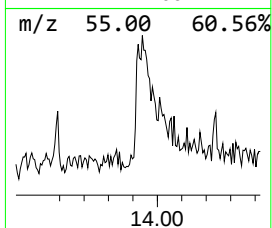
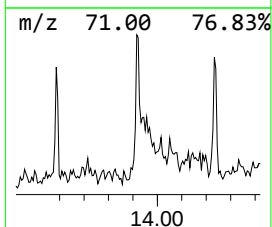
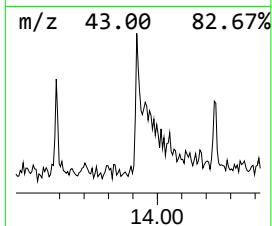
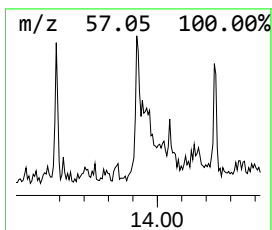
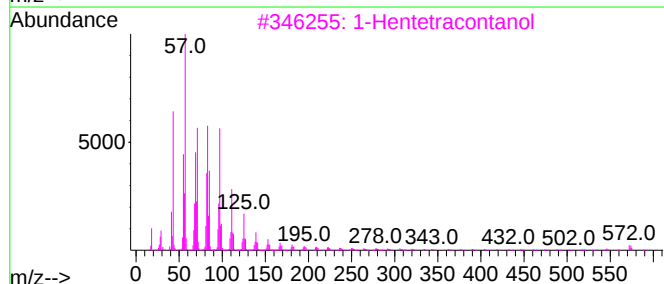
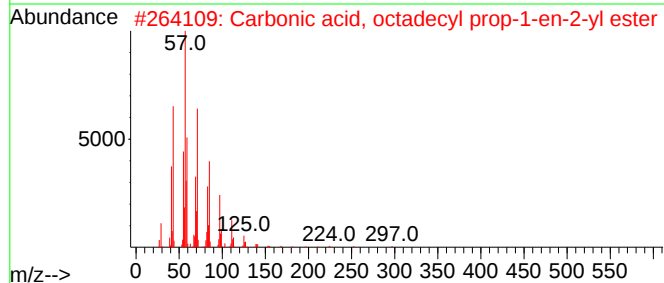
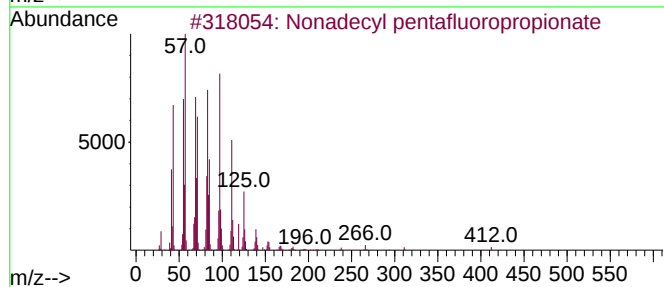
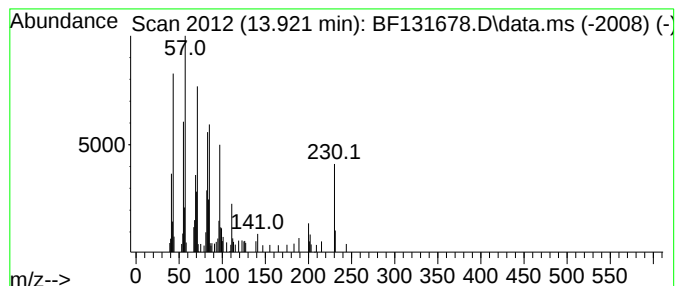
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.921 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	4.38 ng	115012	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	49
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	49
3			1-Hentetracontanol	593	C41H84O	040710-42-7	46
4			Octacosyl propyl ether	452	C31H64O	1000406-28-5	43
5			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131678.D
Acq On : 16 Dec 2022 21:28
Operator : CG\JU
Sample : N6037-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-26-(2-4)

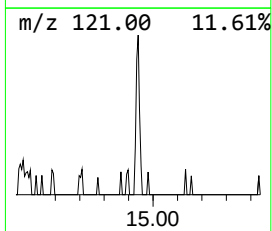
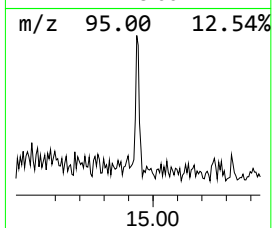
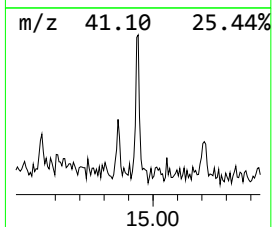
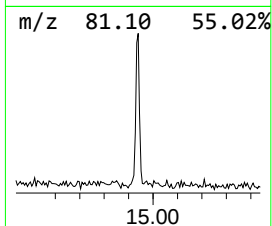
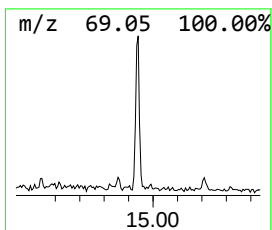
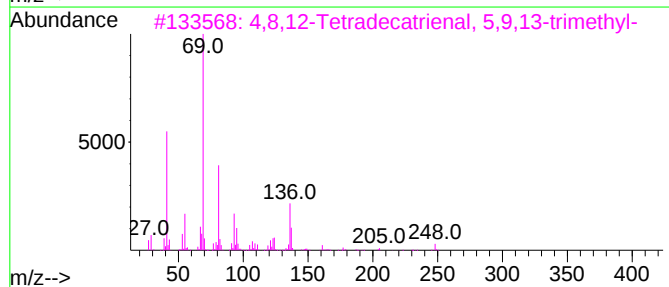
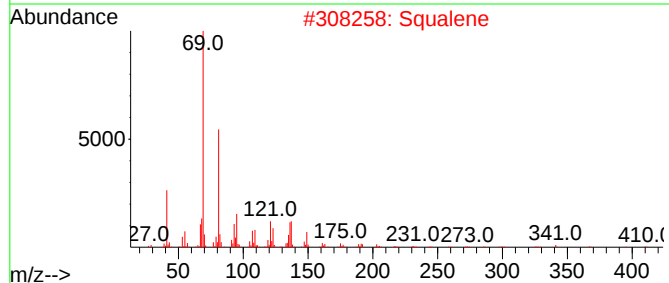
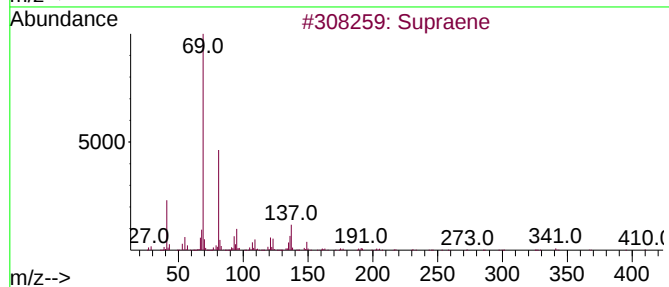
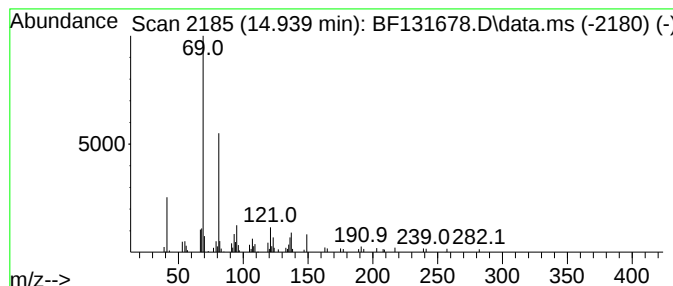
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.31 ng	52145	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	86
2			Squalene	410	C30H50	000111-02-4	80
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			3,7,11-Tridecatrienitrile, 4,8-...	231	C16H25N	006006-01-5	72
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131678.D
Acq On : 16 Dec 2022 21:28
Operator : CG\JU
Sample : N6037-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-26-(2-4)

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...	2.134	23.4	ng	539867	1	6.881	460965	20.0
3-Penten-2-one,...	4.457	8.4	ng	192740	1	6.881	460965	20.0
2-Pentanone, 4-...	5.081	19.8	ng	455417	1	6.881	460965	20.0
Benzophenone	10.645	2.8	ng	93383	3	9.933	663948	20.0
unknown13.921	13.921	4.4	ng	115012	5	14.080	524806	20.0
Supraene	14.939	2.3	ng	52145	6	15.580	451891	20.0