

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131665.D
 Acq On : 16 Dec 2022 14:19
 Operator : CG\JU
 Sample : N6038-15
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-36-(3-5)

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: BF131665.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	17	rVB	361747	452331	18.86%	2.737%
2	5.087	505	510	520	rVB	269370	357751	14.91%	2.164%
3	5.498	575	580	583	rBV	1905691	1866192	77.80%	11.291%
4	6.510	747	752	755	rBV	1956641	1905300	79.43%	11.528%
5	6.881	811	815	818	rBV	575922	466348	19.44%	2.822%
6	7.445	906	911	914	rBV	1286558	1224160	51.03%	7.407%
7	8.169	1030	1034	1037	rBV	732552	582129	24.27%	3.522%
8	9.251	1213	1218	1221	rBV	2793161	2299146	95.85%	13.910%
9	9.933	1330	1334	1337	rBV	849556	684418	28.53%	4.141%
10	10.651	1452	1456	1459	rBV	446209	336309	14.02%	2.035%
11	10.727	1464	1469	1472	rBV	1783827	1476890	61.57%	8.936%
12	11.427	1584	1588	1591	rBV	930117	732764	30.55%	4.433%
13	11.957	1675	1678	1681	rBV2	67006	63959	2.67%	0.387%
14	12.204	1717	1720	1723	rBV	225137	170899	7.12%	1.034%
15	12.645	1792	1795	1798	rVB	65805	53589	2.23%	0.324%
16	12.874	1828	1834	1839	rVB2	50201	50121	2.09%	0.303%
17	13.021	1855	1859	1862	rBV	2648878	2398762	100.00%	14.513%
18	13.945	2008	2016	2032	rBV6	60038	275818	11.50%	1.669%
19	14.080	2034	2039	2042	rBV	616738	523860	21.84%	3.170%
20	14.604	2123	2128	2137	rBV	12459	47113	1.96%	0.285%
21	14.939	2181	2185	2189	rBV	41449	41276	1.72%	0.250%
22	15.139	2216	2219	2222	rBV	22748	30191	1.26%	0.183%
23	15.215	2228	2232	2236	rVB	27394	32171	1.34%	0.195%
24	15.586	2289	2295	2304	rBV	329657	426748	17.79%	2.582%
25	16.068	2371	2377	2383	rVB3	17491	29896	1.25%	0.181%

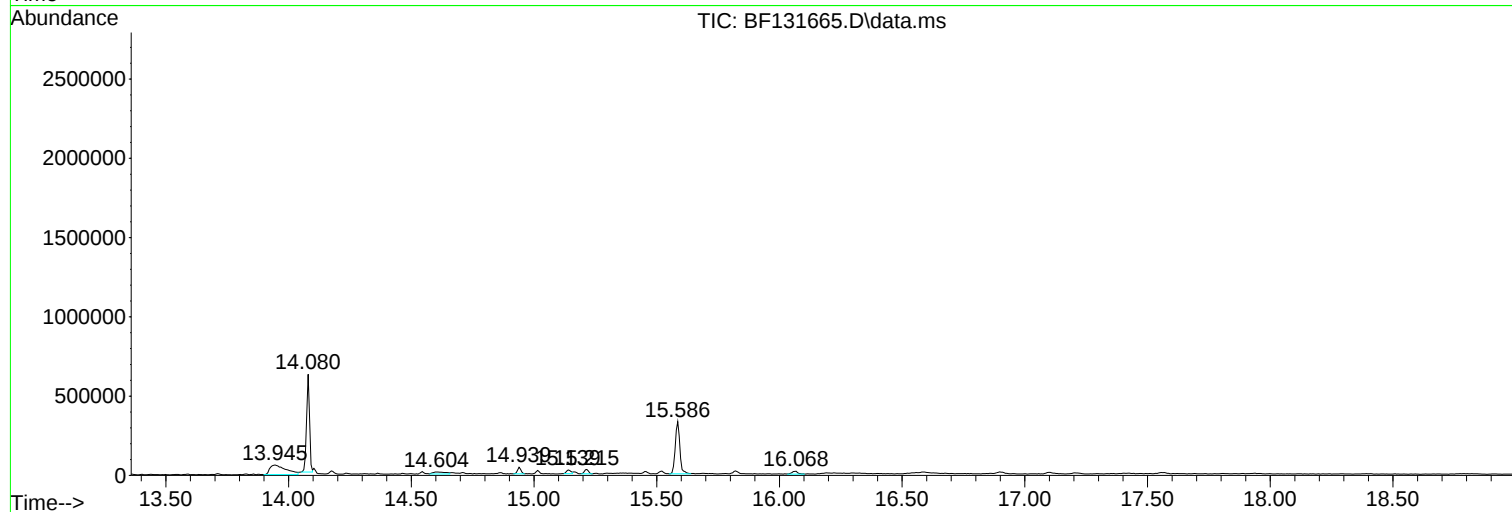
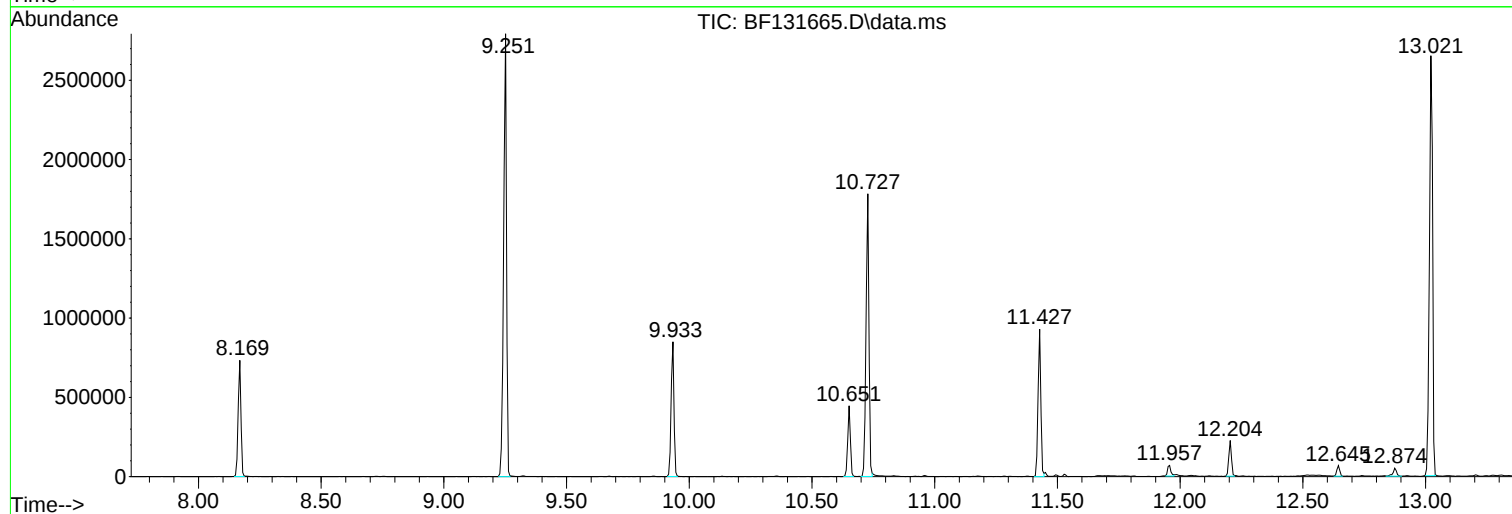
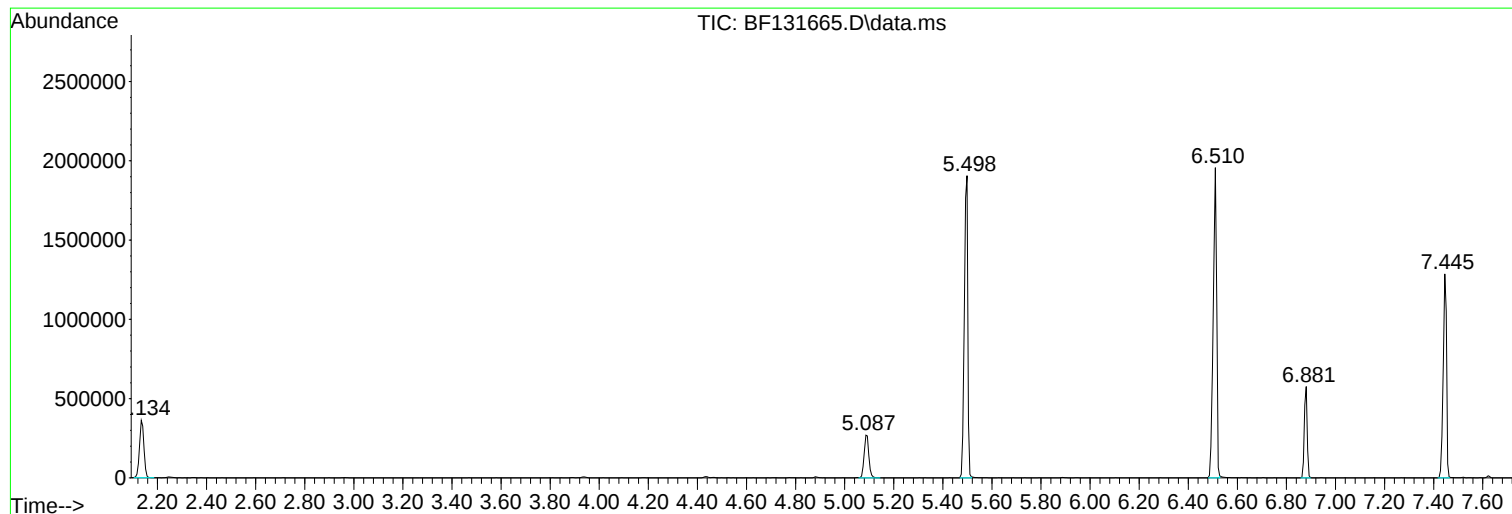
Sum of corrected areas: 16528141

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

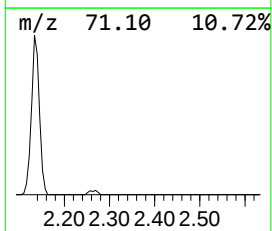
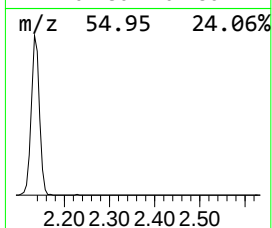
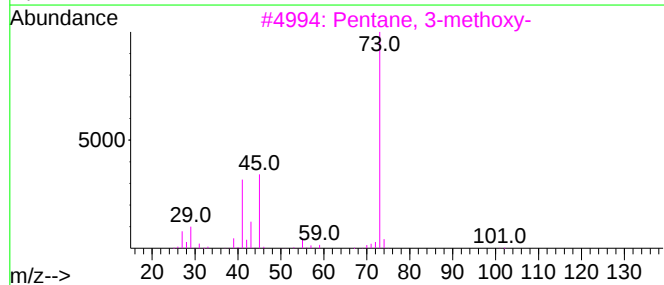
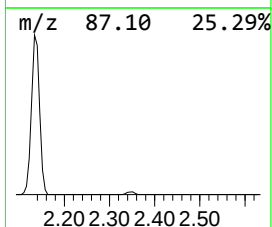
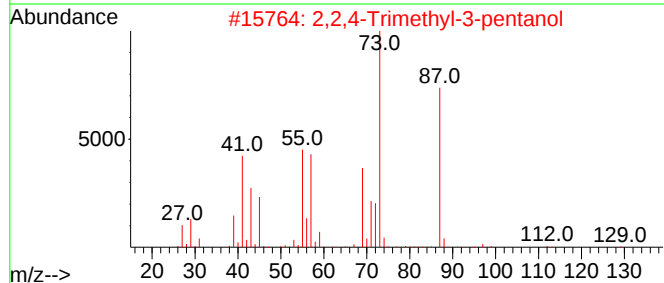
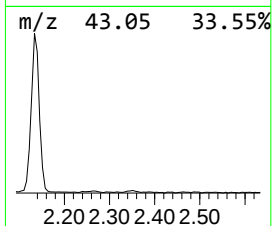
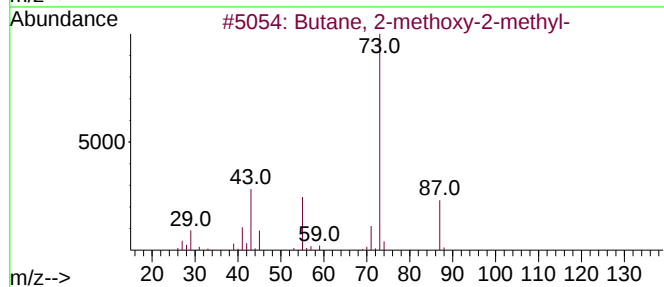
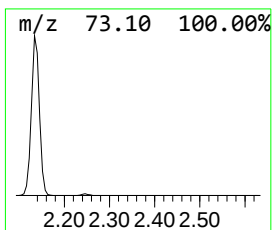
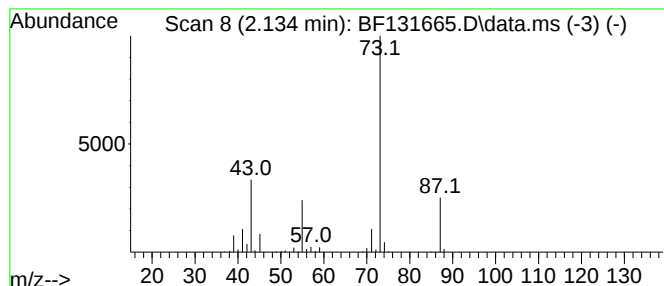
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	19.40 ng	452331	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

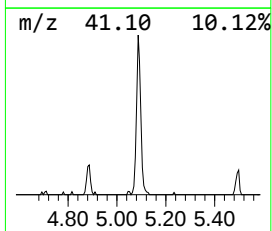
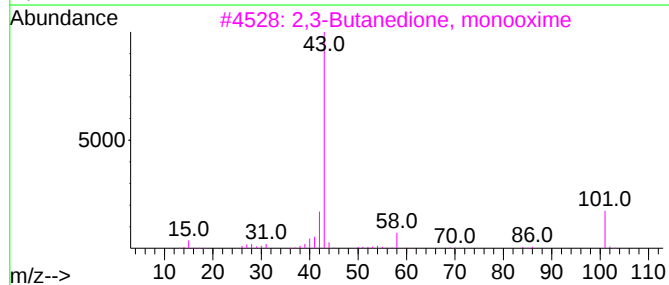
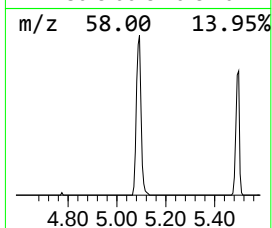
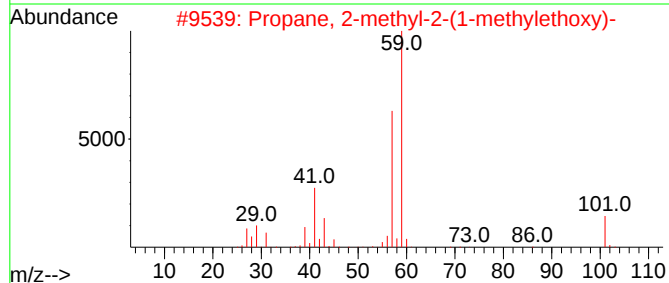
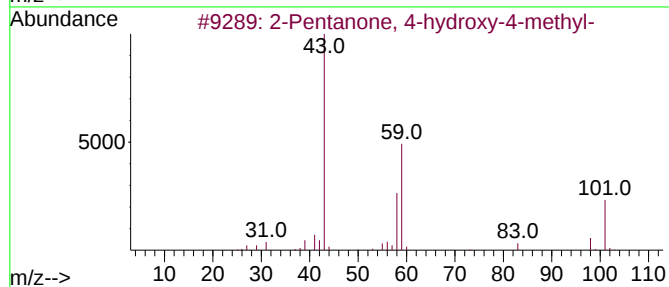
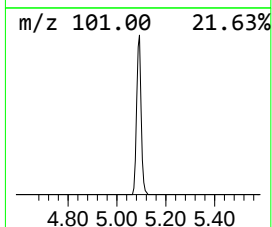
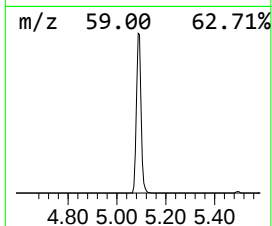
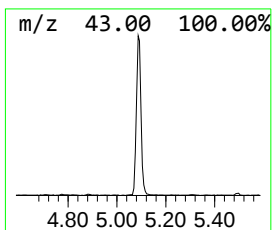
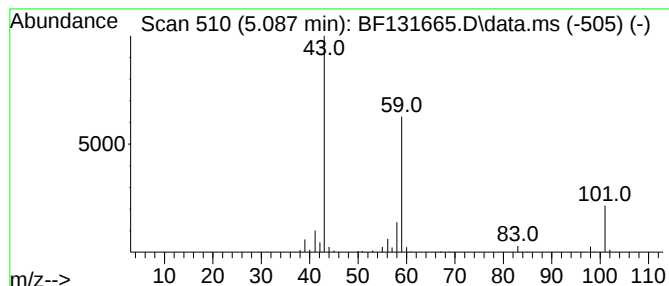
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	15.34 ng	357751	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	72
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

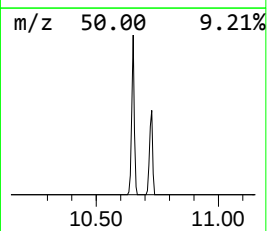
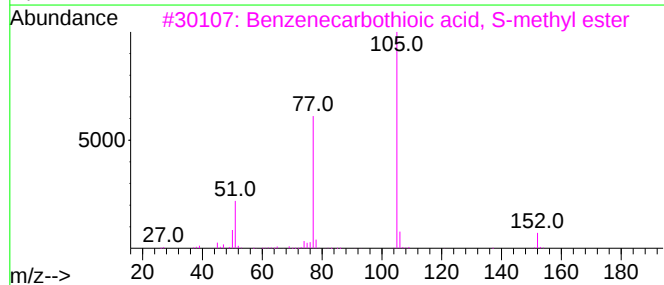
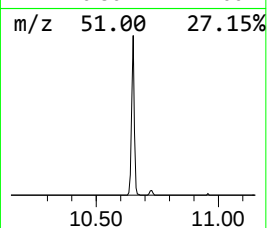
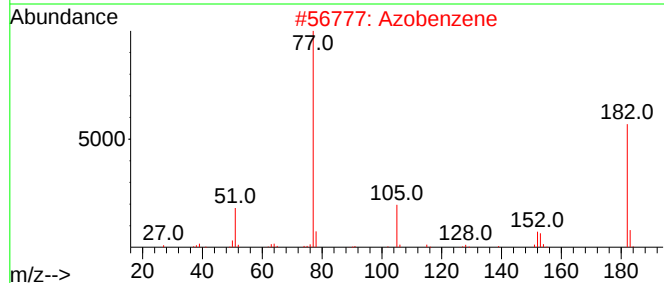
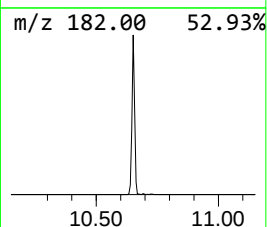
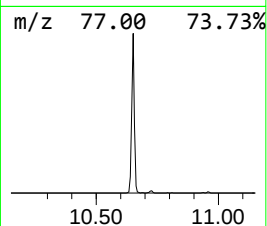
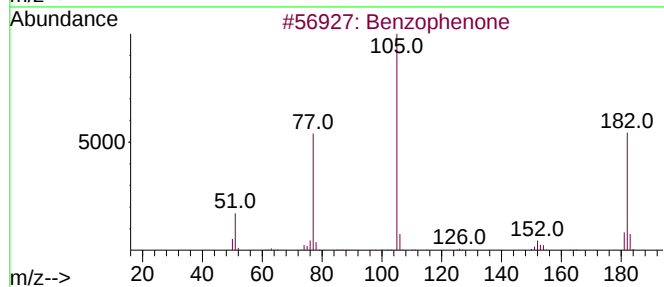
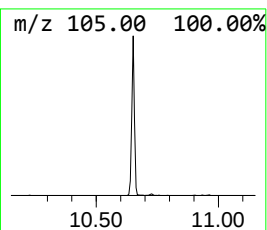
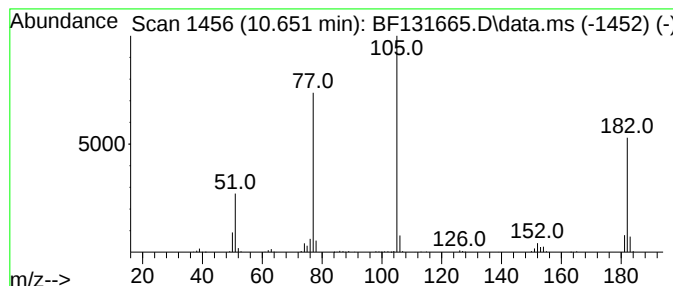
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	9.83 ng	336309	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	53
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

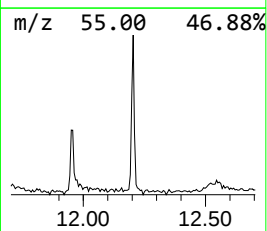
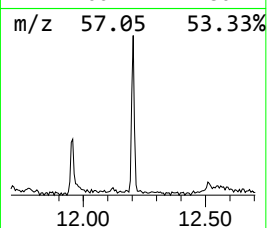
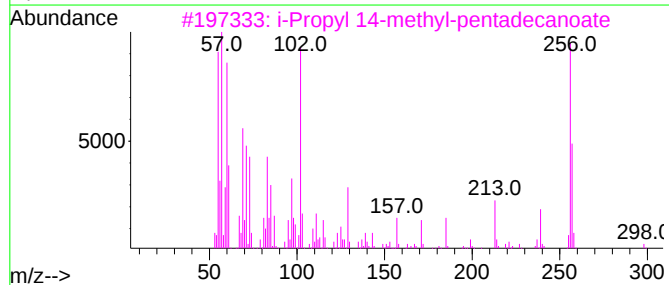
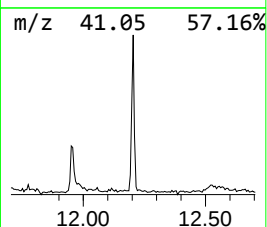
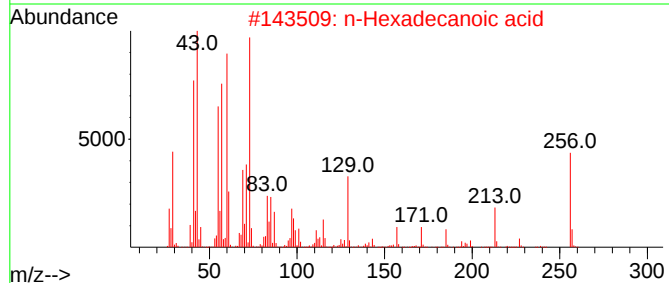
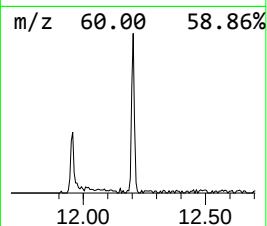
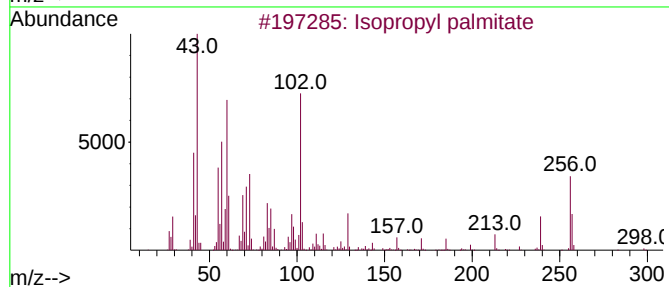
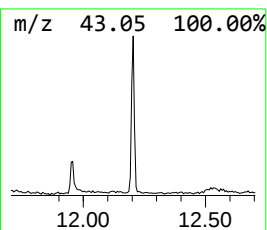
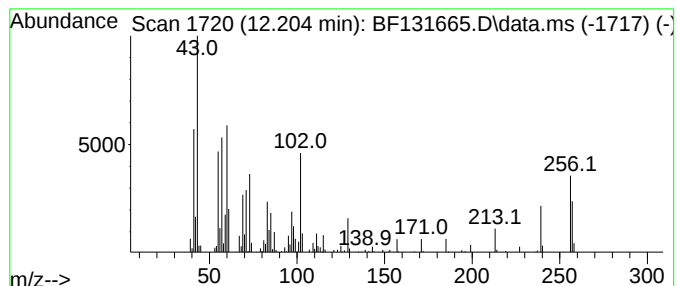
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Isopropyl palmitate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	4.66 ng	170899	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl palmitate	298	C19H38O2	000142-91-6	86
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3		i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	58
4		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	35
5		Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1010126-15-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

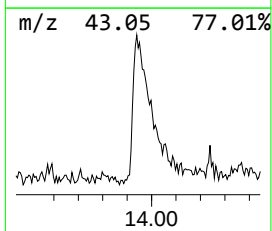
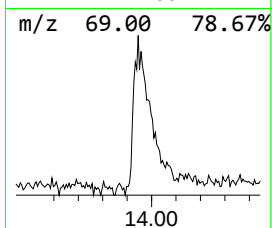
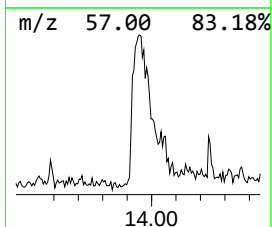
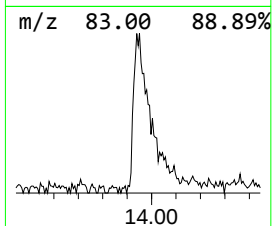
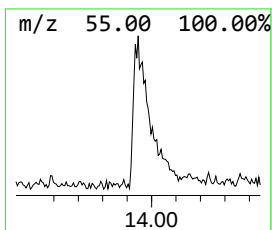
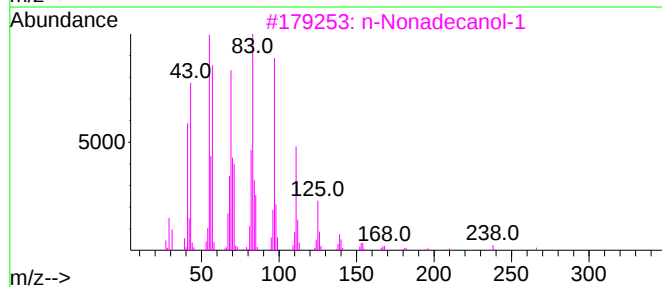
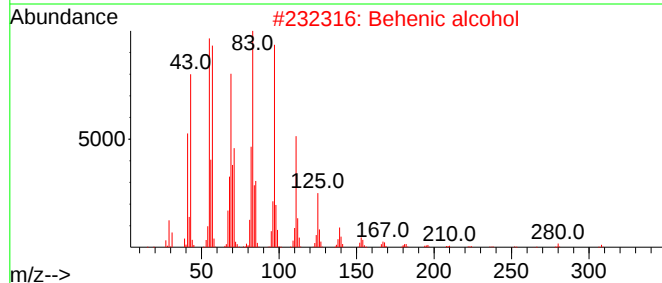
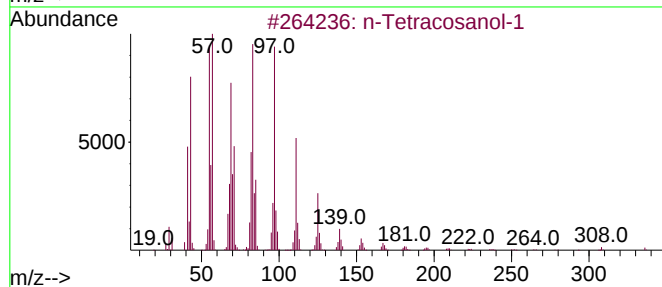
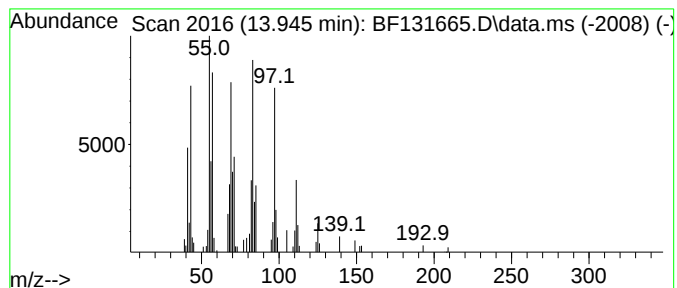
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	10.53 ng	275818	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131665.D
Acq On : 16 Dec 2022 14:19
Operator : CG\JU
Sample : N6038-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-36-(3-5)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	19.4	ng	452331	1	6.881	466348	20.0
2-Pentanone, 4-...	5.087	15.3	ng	357751	1	6.881	466348	20.0
Benzophenone	10.651	9.8	ng	336309	3	9.933	684418	20.0
Isopropyl palmi...	12.204	4.7	ng	170899	4	11.427	732764	20.0
n-Tetracosanol-1	13.945	10.5	ng	275818	5	14.080	523860	20.0