

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
 Data File : BF127209.D
 Acq On : 04 Mar 2022 19:10
 Operator : CG\JU
 Sample : N1793-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127209.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.098	475	478	482	rVB	65228	65006	1.86%	0.350%
2	5.498	543	546	555	rBV2	811526	794023	22.68%	4.280%
3	5.904	611	615	623	rVB	116377	106610	3.05%	0.575%
4	6.504	714	717	729	rVB	412148	450880	12.88%	2.430%
5	6.875	776	780	784	rBV	729623	580931	16.59%	3.131%
6	7.022	802	805	815	rVB	324966	278671	7.96%	1.502%
7	7.445	871	877	879	rBV	1805484	1955693	55.86%	10.541%
8	7.610	901	905	908	rVB	75651	68318	1.95%	0.368%
9	8.157	994	998	1002	rBV	929360	792345	22.63%	4.271%
10	8.739	1091	1097	1101	rBV	37469	39739	1.14%	0.214%
11	9.234	1176	1181	1185	rBV	3443969	3501055	100.00%	18.870%
12	9.304	1189	1193	1196	rVV	72794	58789	1.68%	0.317%
13	9.916	1291	1297	1301	rVB	1003997	919406	26.26%	4.955%
14	10.710	1428	1432	1436	rBV	1958666	1727475	49.34%	9.311%
15	11.410	1547	1551	1554	rBV	1170251	926803	26.47%	4.995%
16	11.792	1612	1616	1619	rVB	468986	425249	12.15%	2.292%
17	11.822	1619	1621	1624	rVB	48285	37943	1.08%	0.205%
18	12.498	1733	1736	1741	rVB	108467	91734	2.62%	0.494%
19	12.998	1816	1821	1824	rBV	3556799	3459135	98.80%	18.644%
20	13.280	1865	1869	1872	rVB	166603	137488	3.93%	0.741%
21	13.916	1974	1977	1979	rBV	41111	40632	1.16%	0.219%
22	13.968	1979	1986	1988	rBV3	65748	130948	3.74%	0.706%
23	14.057	1997	2001	2004	rVB	820548	714133	20.40%	3.849%
24	14.151	2011	2017	2023	rBV	370274	391066	11.17%	2.108%
25	14.815	2126	2130	2135	rBV	49582	66333	1.89%	0.358%
26	15.010	2157	2163	2166	rBV	35967	45329	1.29%	0.244%
27	15.163	2185	2189	2193	rVB2	35417	43539	1.24%	0.235%
28	15.545	2249	2254	2260	rVB	489495	606263	17.32%	3.268%
29	15.992	2326	2330	2335	rVB	34784	49116	1.40%	0.265%
30	16.509	2411	2418	2422	rBV4	26179	49187	1.40%	0.265%

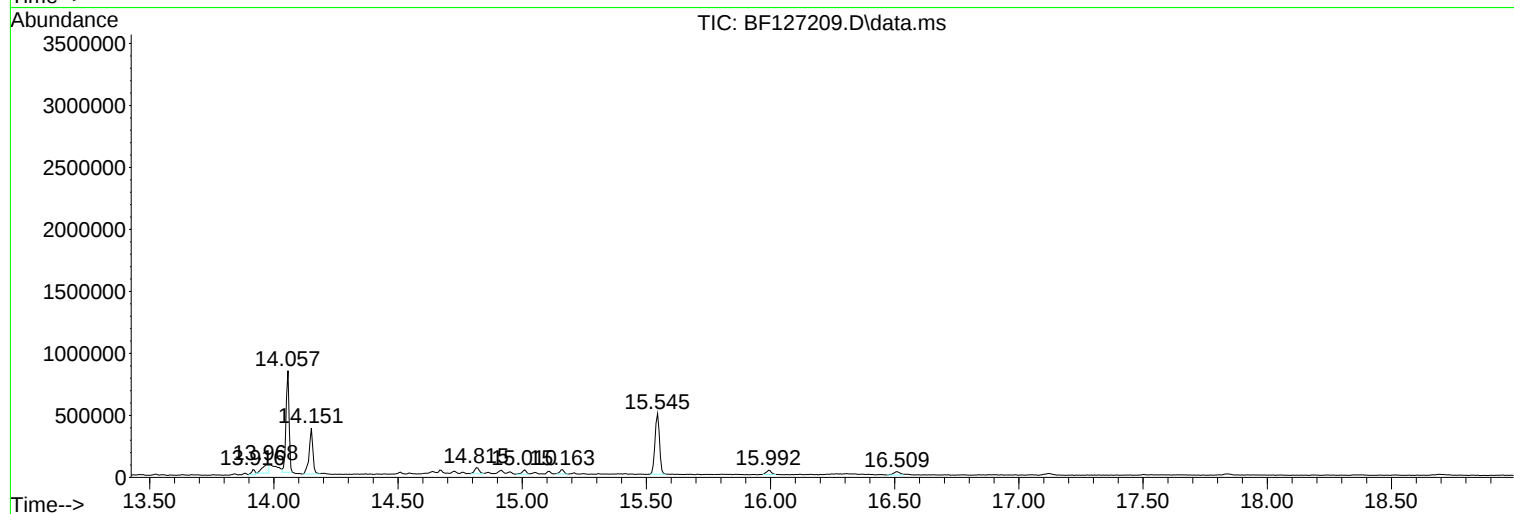
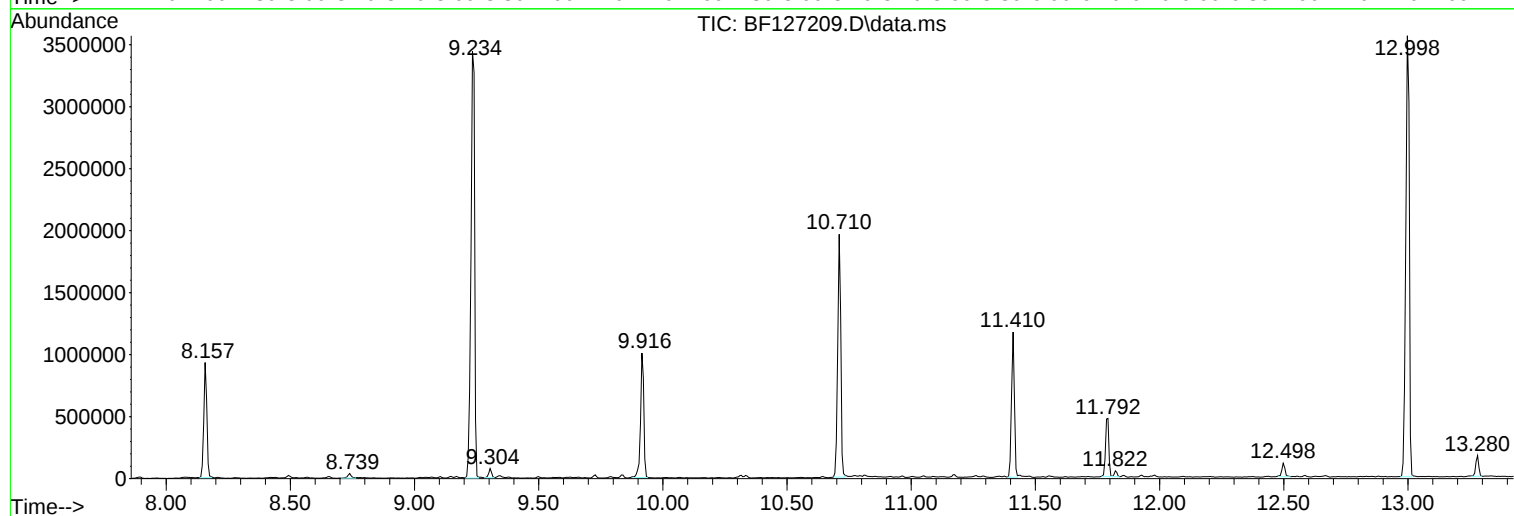
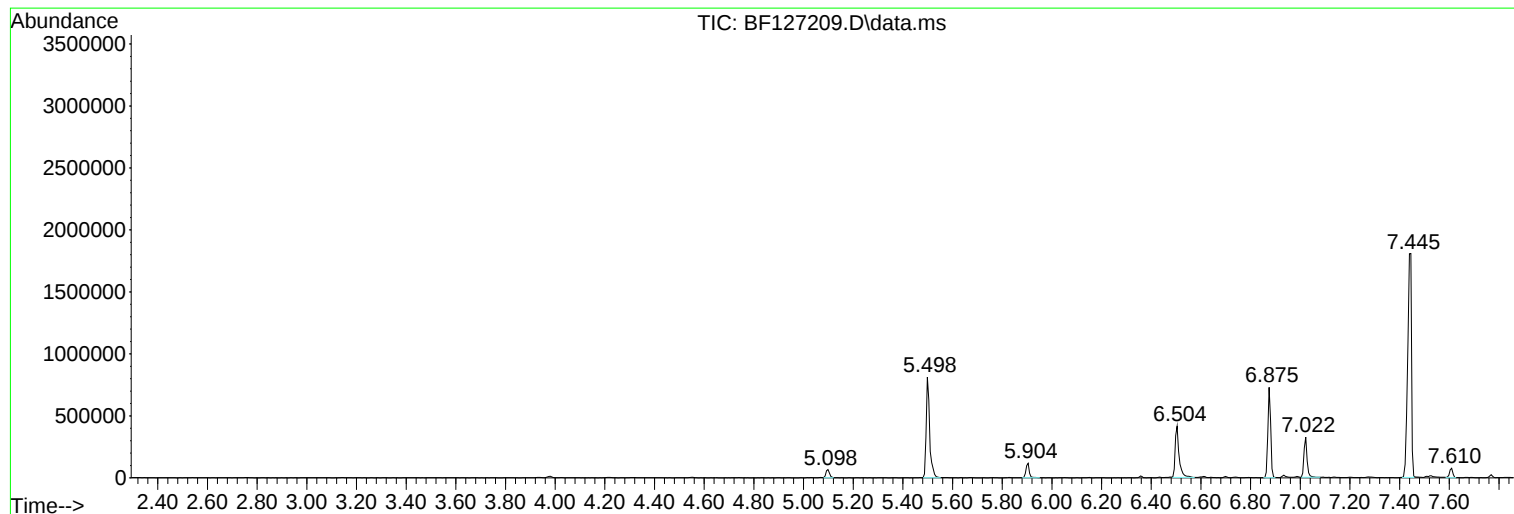
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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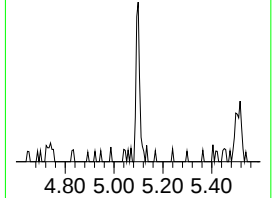
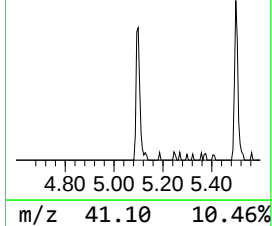
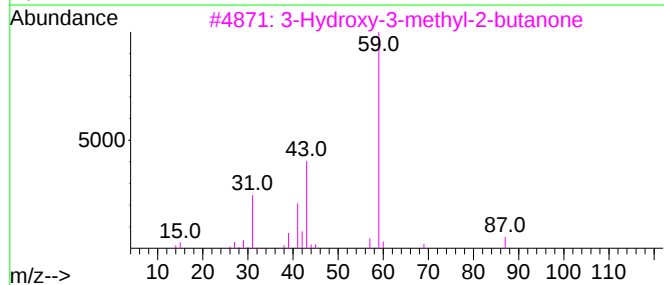
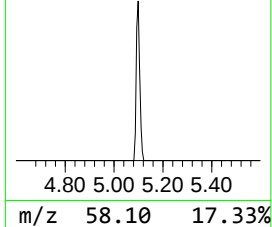
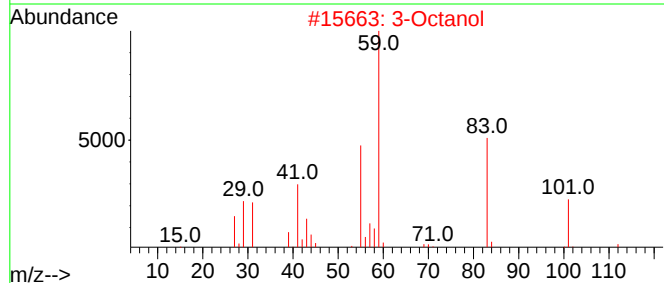
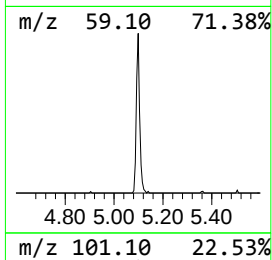
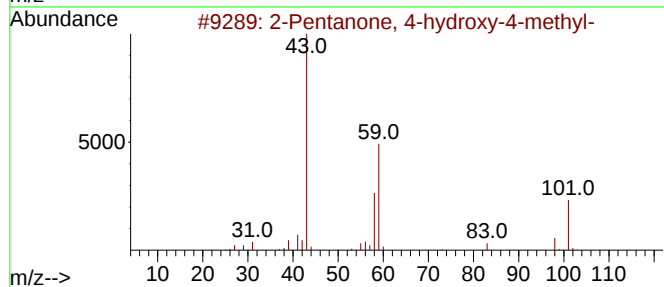
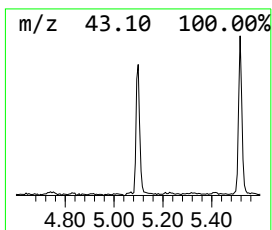
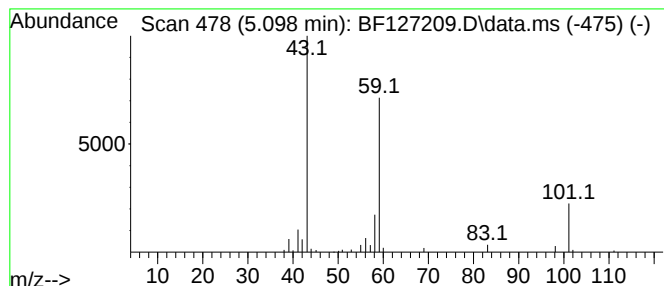
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	2.24 ng	65006	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	Acetone	58	C3H6O	000067-64-1	10		



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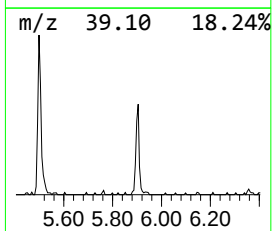
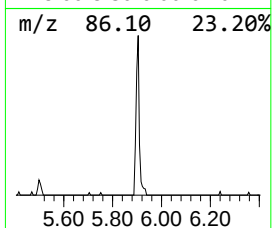
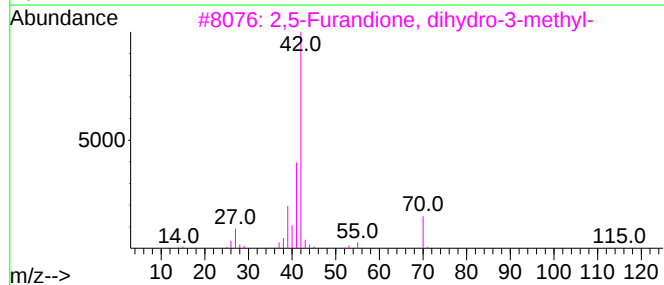
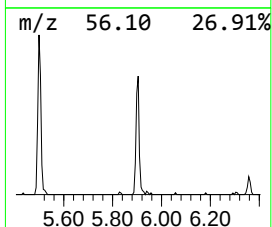
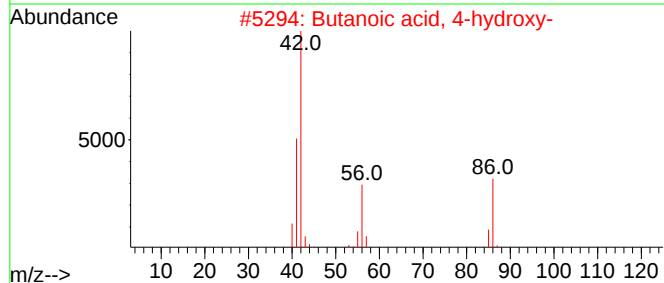
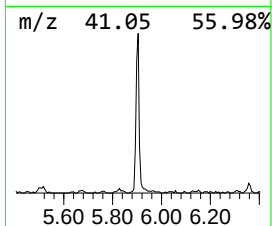
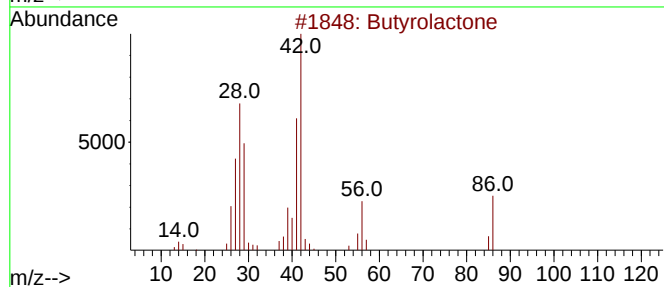
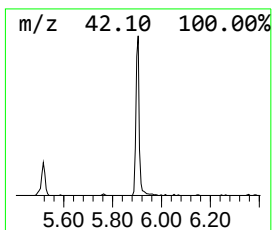
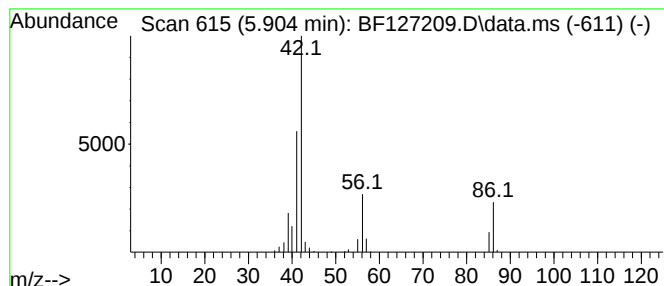
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butyrolactone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.904	3.67 ng	106610	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyrolactone	86	C4H6O2	000096-48-0	90
2			Butanoic acid, 4-hydroxy-	104	C4H8O3	000591-81-1	83
3			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	38
4			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	16
5			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	14



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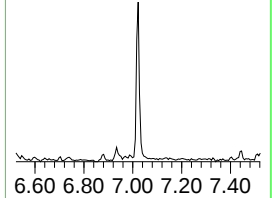
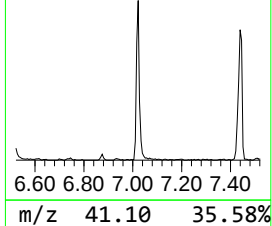
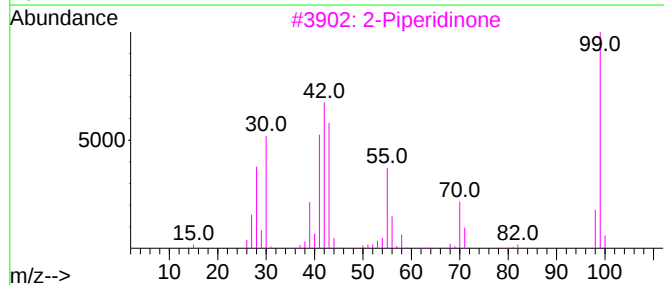
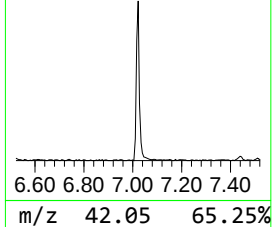
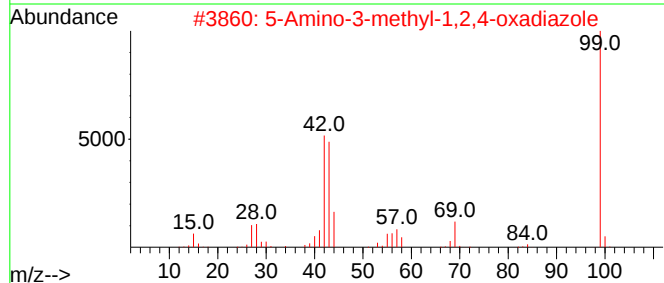
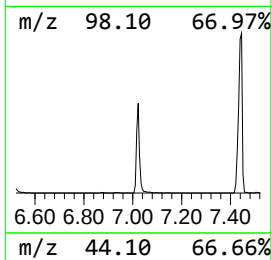
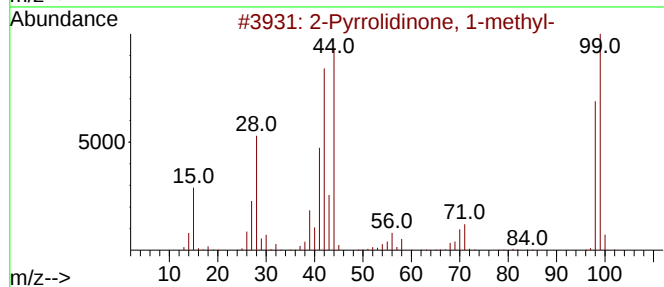
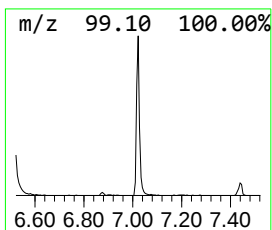
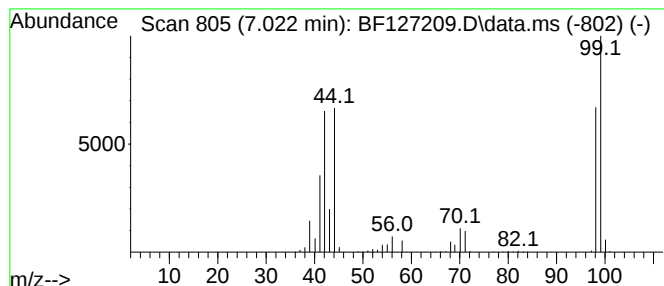
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.022	9.59 ng	278671	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	94
2			5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	43
3			2-Piperidinone	99	C5H9NO	000675-20-7	40
4			1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	25
5			Imidosulfurous difluoride, methyl-	99	CH3F2NS	000758-20-3	25



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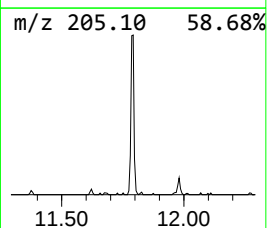
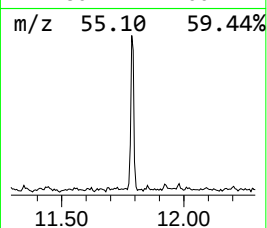
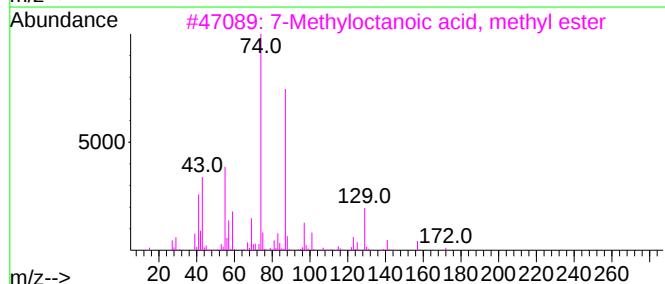
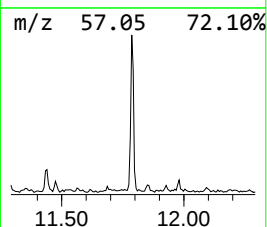
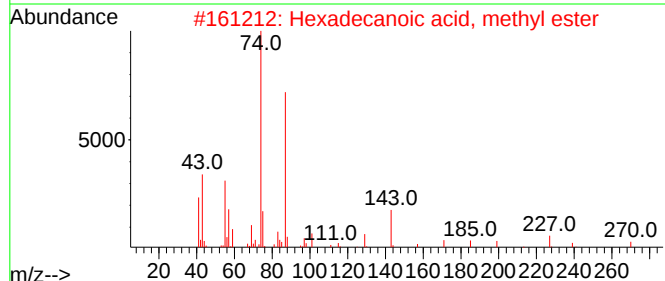
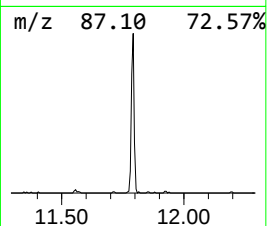
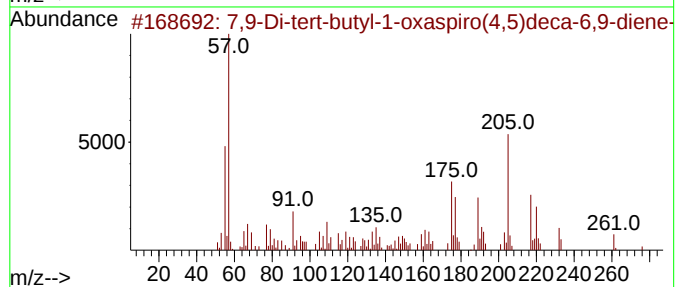
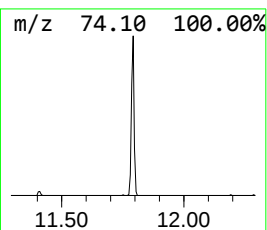
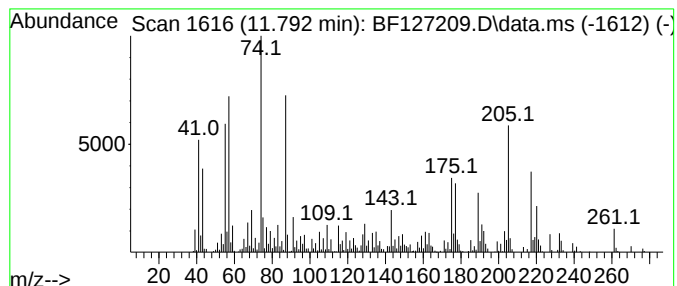
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.792	9.18 ng	425249	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	96
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	83
3	7-Methyloctanoic acid, methyl ester	172	C10H20O2	005129-53-3	42
4	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	38
5	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	30



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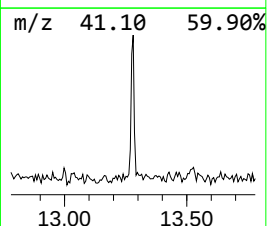
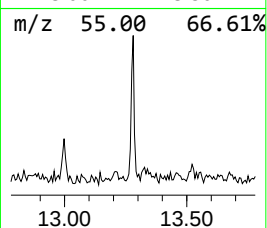
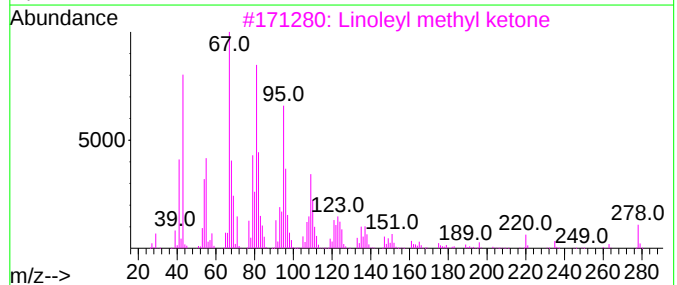
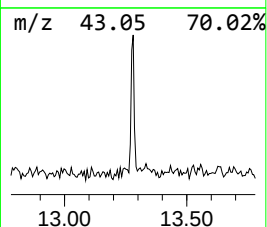
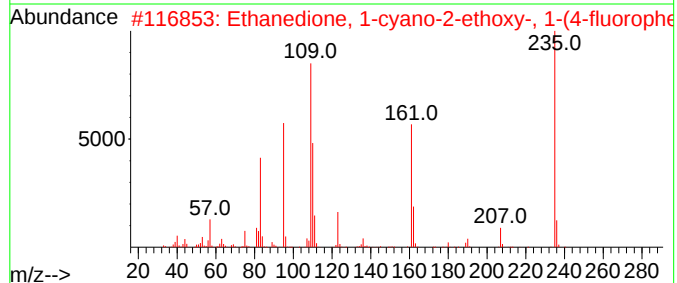
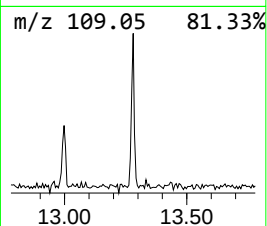
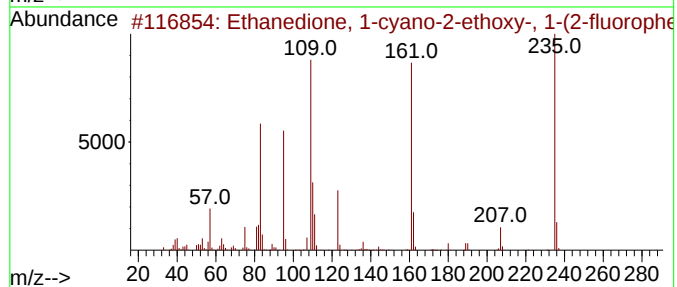
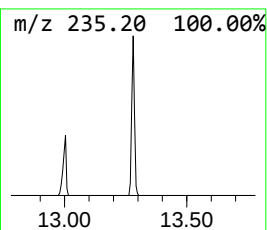
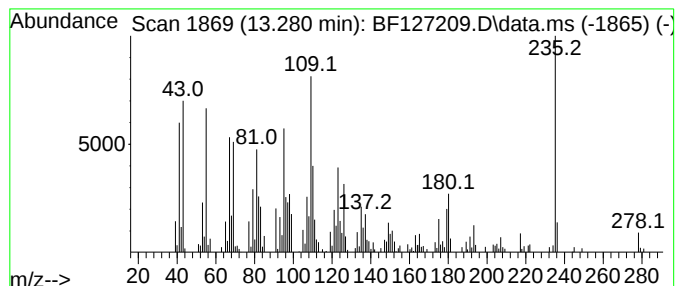
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Peak Number 5 Ethanedione, 1-cyano-2-etho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.280	3.85 ng	137488	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanedione, 1-cyano-2-ethoxy-, ...	235	C11H10FN3O2	326909-08-4	68
2			Ethanedione, 1-cyano-2-ethoxy-, ...	235	C11H10FN3O2	263256-02-6	62
3			Linoleyl methyl ketone	278	C19H34O	029204-24-8	40
4			(1S,5R,10S)-1,5,8,8-Tetramethylb...	236	C15H24O2	088010-66-6	38
5			3-Tetradecyne	194	C14H26	060212-32-0	30



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SB-5

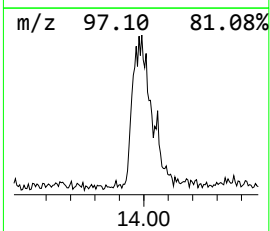
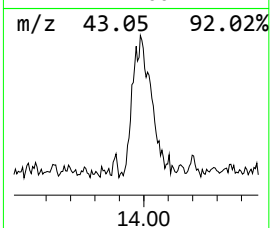
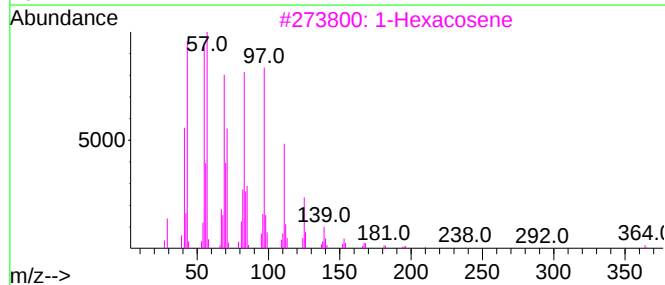
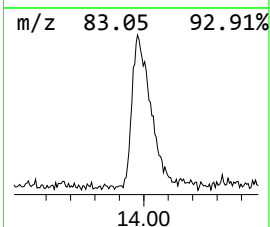
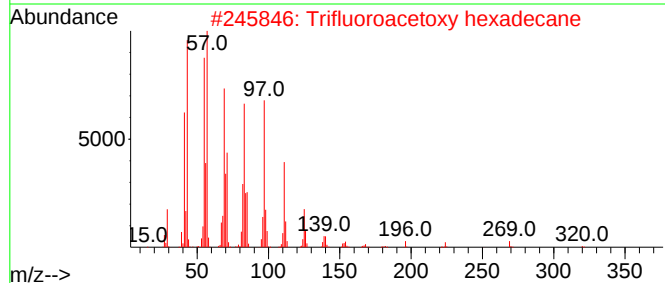
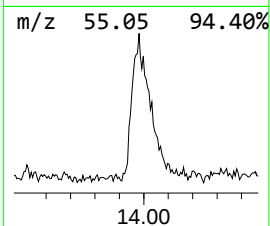
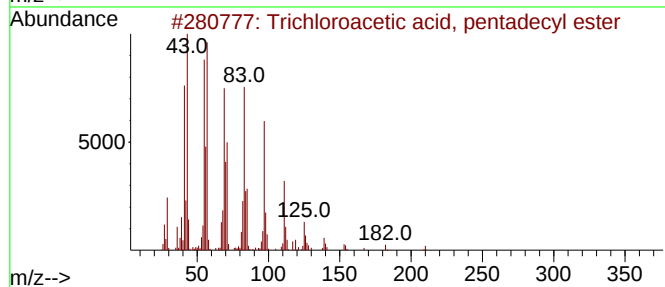
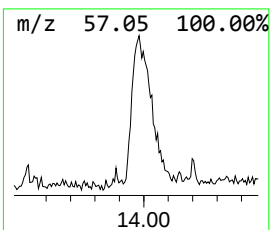
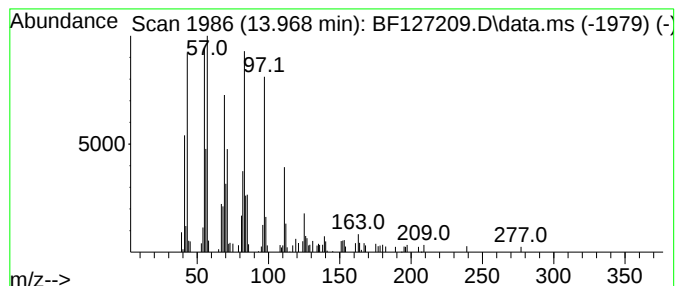
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	3.67 ng	130948	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127209.D
Acq On : 04 Mar 2022 19:10
Operator : CG\JU
Sample : N1793-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5

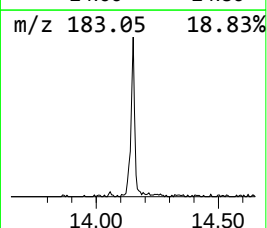
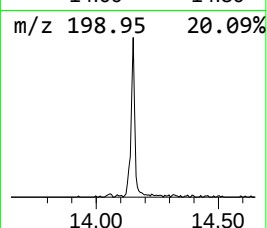
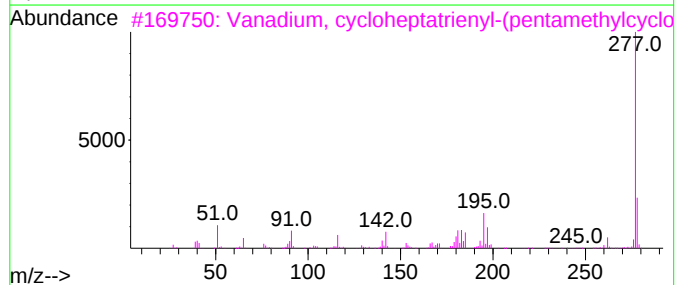
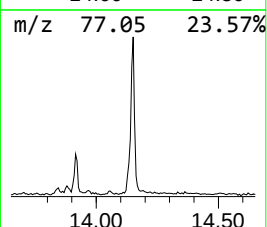
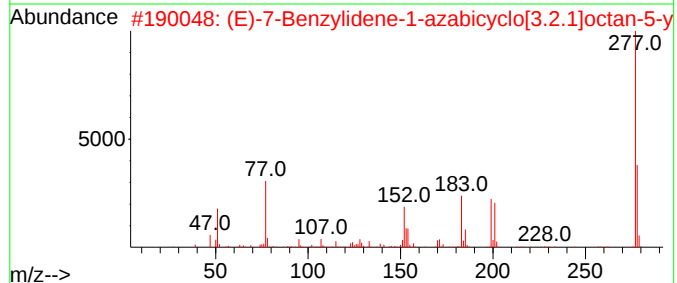
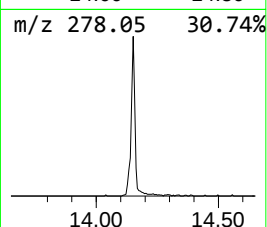
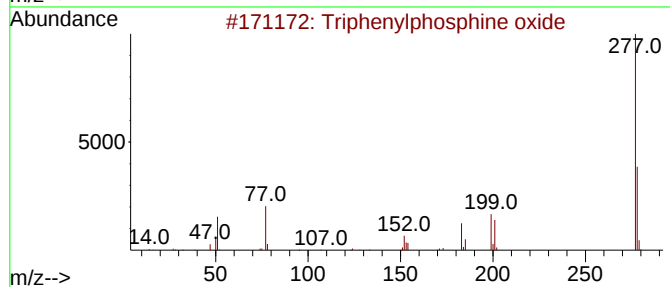
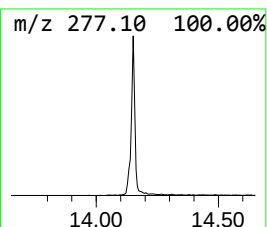
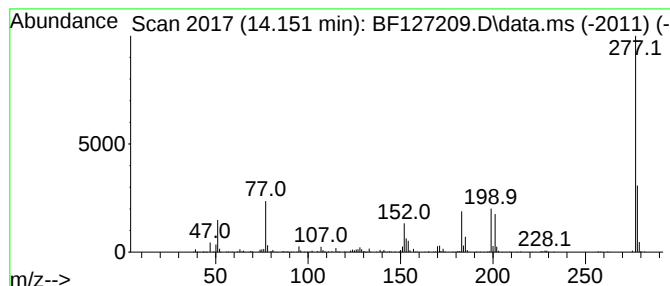
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	10.95 ng	391066	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	70
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127209.D
Acq On : 04 Mar 2022 19:10
Operator : CG\JU
Sample : N1793-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5

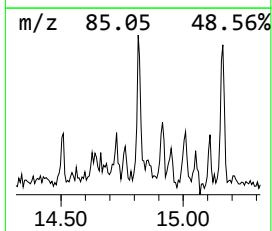
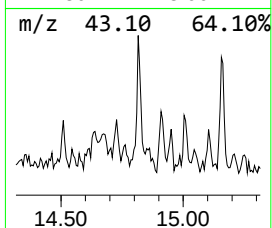
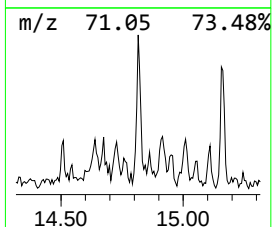
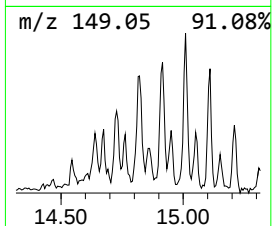
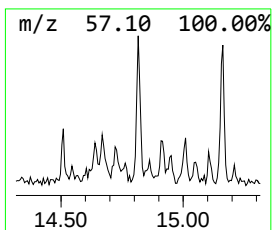
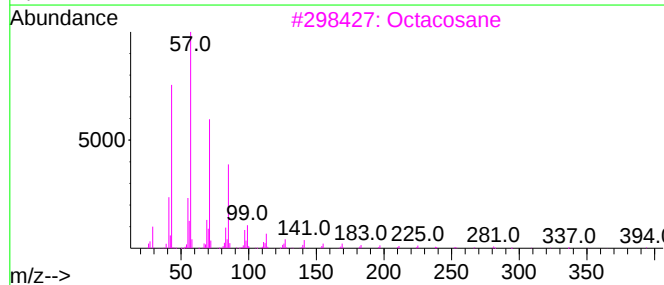
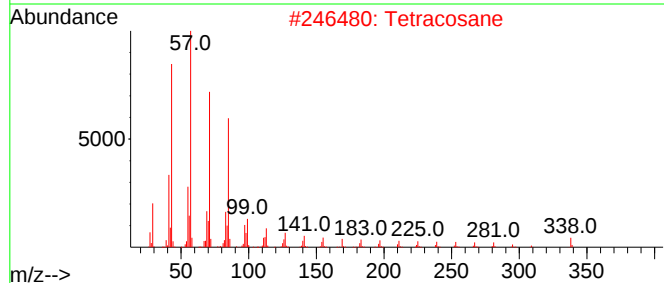
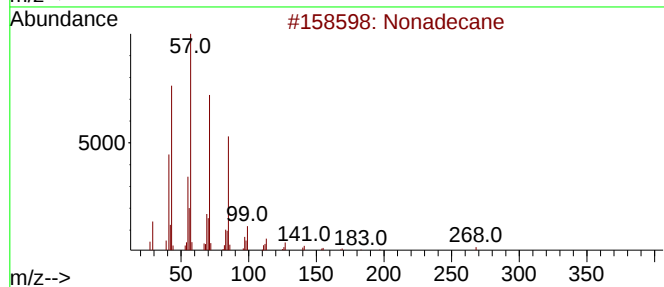
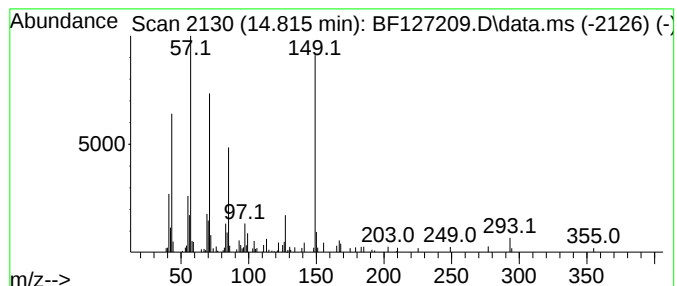
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.816 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.19 ng	66333	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	49
2			Tetracosane	338	C24H50	000646-31-1	49
3			Octacosane	394	C28H58	000630-02-4	49
4			10-Methylnonadecane	282	C20H42	056862-62-5	49
5			Hexadecane	226	C16H34	000544-76-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127209.D
Acq On : 04 Mar 2022 19:10
Operator : CG\JU
Sample : N1793-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
2-Pentanone, 4-...	5.098	2.2	ng	65006	1	6.875	580931	20.0
Butyrolactone	5.904	3.7	ng	106610	1	6.875	580931	20.0
2-Pyrrolidinone...	7.022	9.6	ng	278671	1	6.875	580931	20.0
7,9-Di-tert-but...	11.792	9.2	ng	425249	4	11.410	926803	20.0
Ethanedione, 1-...	13.280	3.9	ng	137488	5	14.057	714133	20.0
Trichloroacetic...	13.969	3.7	ng	130948	5	14.057	714133	20.0
Triphenylphosph...	14.151	10.9	ng	391066	5	14.057	714133	20.0
unknown14.816	14.816	2.2	ng	66333	6	15.545	606263	20.0