

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
 Data File : BF141764.D
 Acq On : 25 Feb 2025 15:06
 Operator : RC/JU
 Sample : Q1421-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-CLAY-CF01-02

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	489	493	508	rVB	36284	65834	2.54%	0.416%
2	5.404	558	563	592	rBV	1531684	2201614	84.81%	13.925%
3	6.422	731	736	765	rBV	1521939	2283290	87.95%	14.442%
4	6.781	792	797	805	rBV	339784	425207	16.38%	2.689%
5	7.345	887	893	905	rBV	1058031	1436381	55.33%	9.085%
6	7.610	933	938	952	rBV	23768	62196	2.40%	0.393%
7	8.063	1010	1015	1034	rVB	393676	557597	21.48%	3.527%
8	9.133	1192	1197	1221	rBV	1940451	2596079	100.00%	16.420%
9	9.816	1307	1313	1327	rBV	442981	620550	23.90%	3.925%
10	10.527	1429	1434	1442	rBV	214328	278775	10.74%	1.763%
11	10.604	1442	1447	1462	rVV	910898	1266940	48.80%	8.013%
12	11.298	1560	1565	1581	rVB	395200	571442	22.01%	3.614%
13	11.833	1650	1656	1676	rBV2	95540	227584	8.77%	1.439%
14	12.621	1784	1790	1810	rBV5	26298	85633	3.30%	0.542%
15	12.880	1829	1834	1846	rBV	1474684	1966348	75.74%	12.437%
16	13.786	1982	1988	2007	rBV2	46546	177187	6.83%	1.121%
17	13.939	2009	2014	2025	rVB	303384	434778	16.75%	2.750%
18	14.686	2136	2141	2148	rBV2	50453	83900	3.23%	0.531%
19	15.386	2254	2260	2269	rBV	276568	469029	18.07%	2.967%

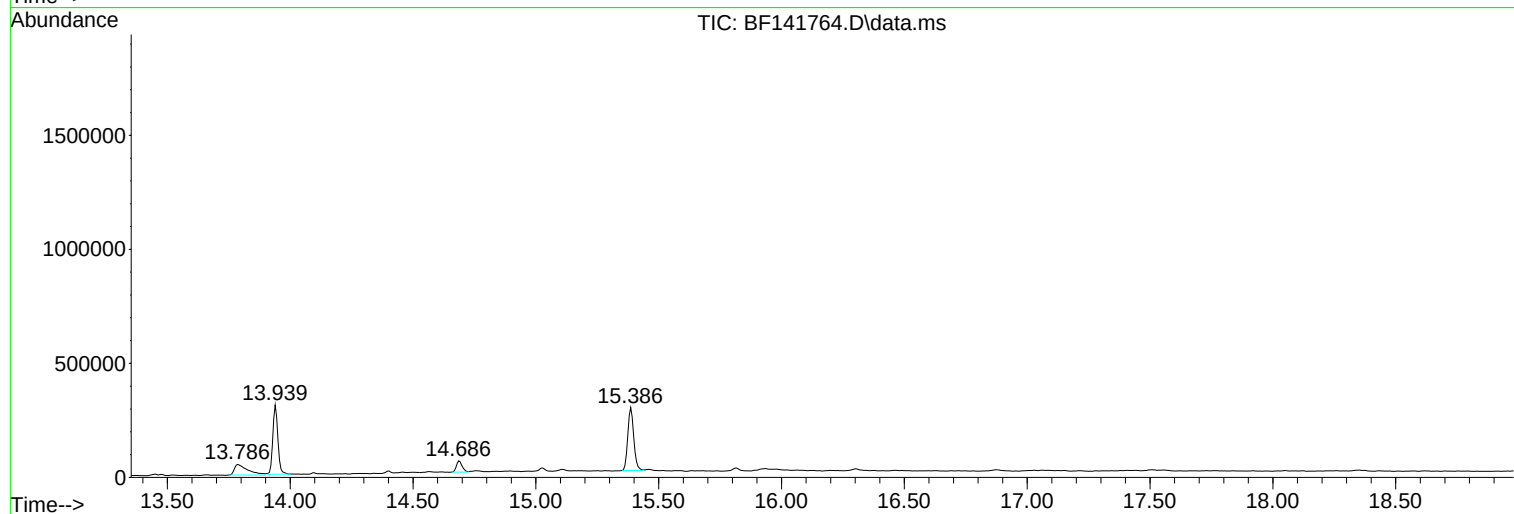
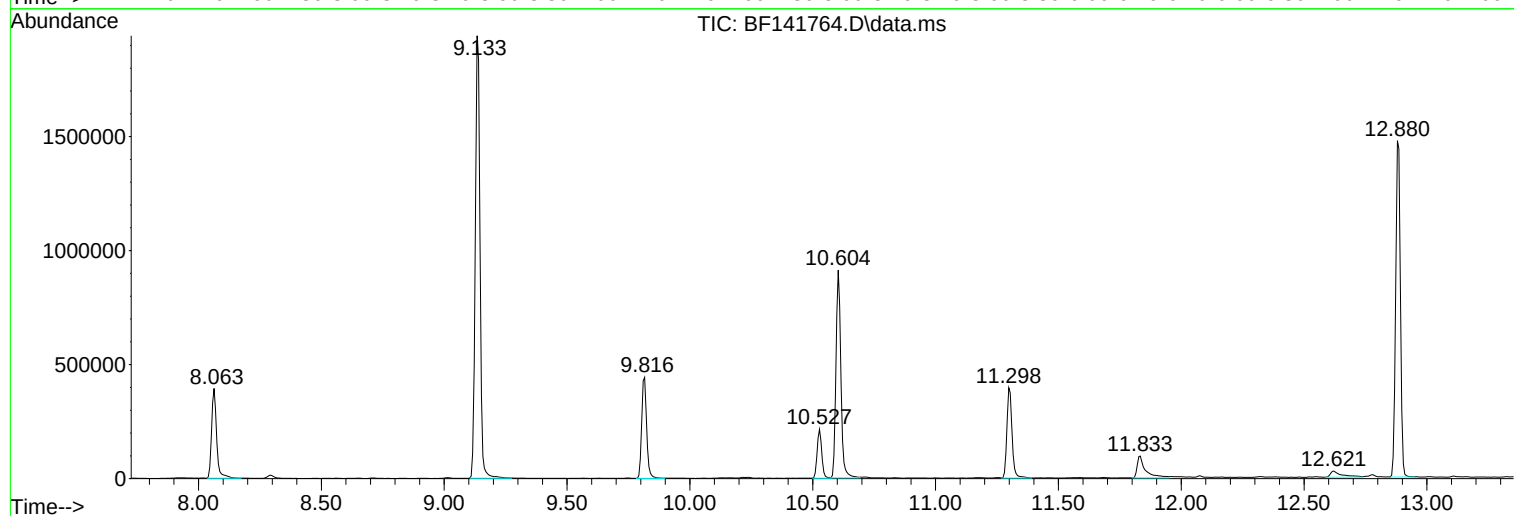
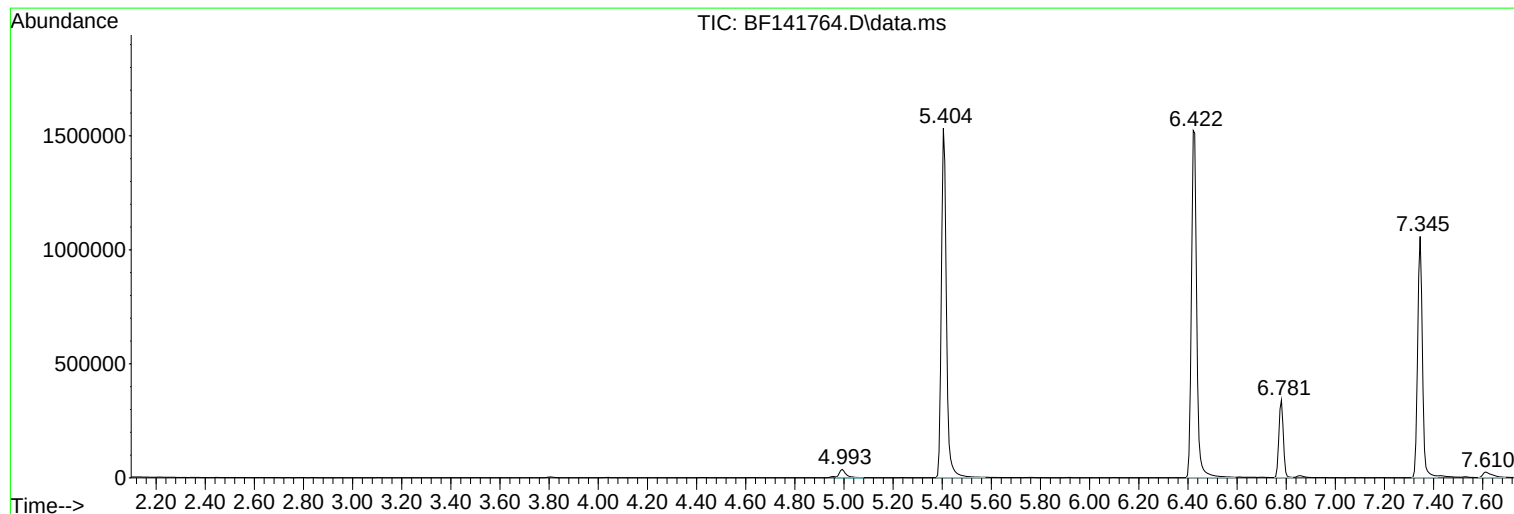
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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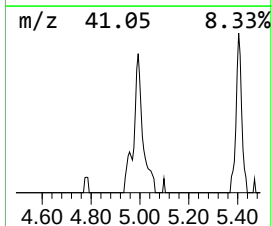
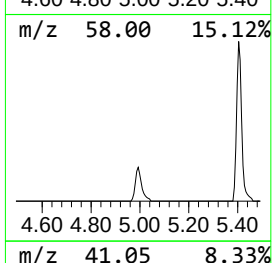
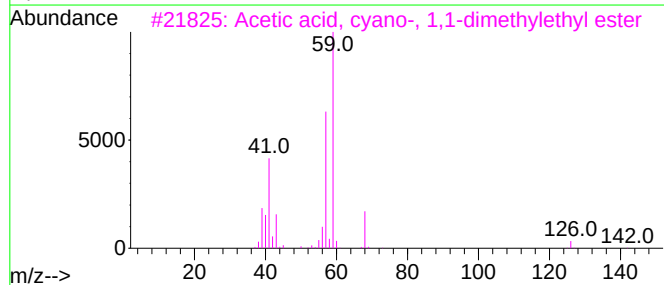
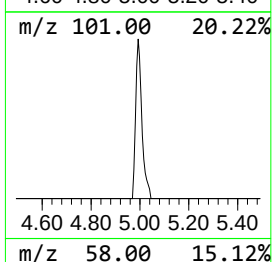
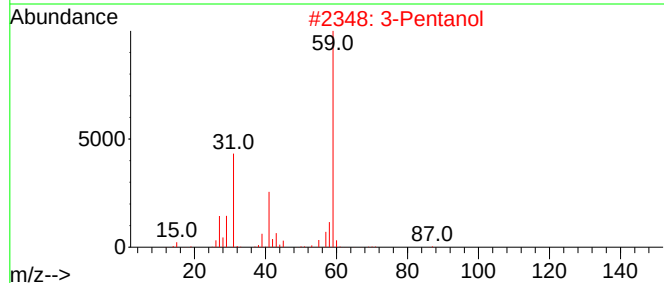
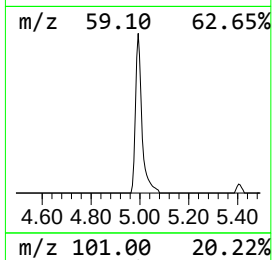
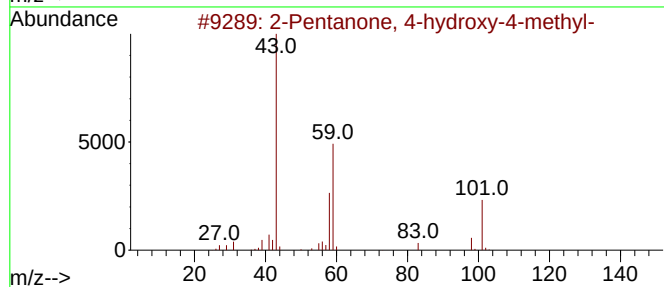
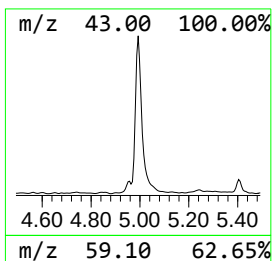
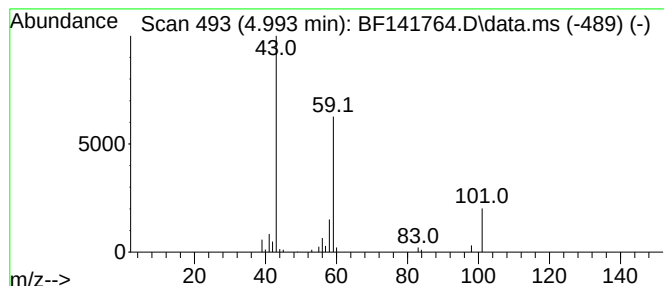
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	3.10 ng	65834	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Pentanol	88	C5H12O	000584-02-1	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		



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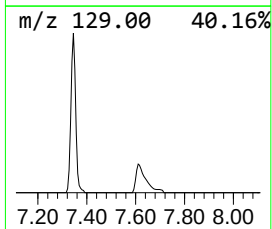
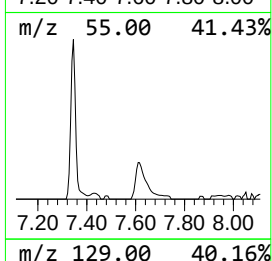
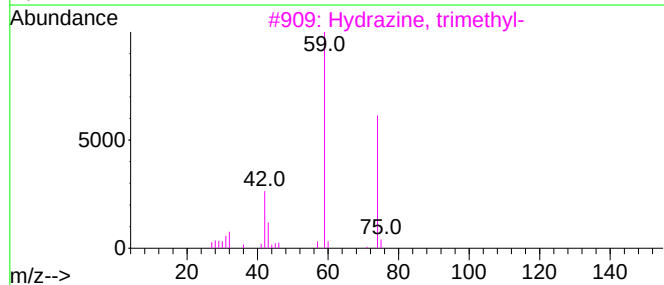
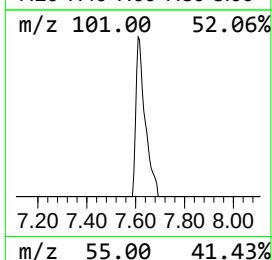
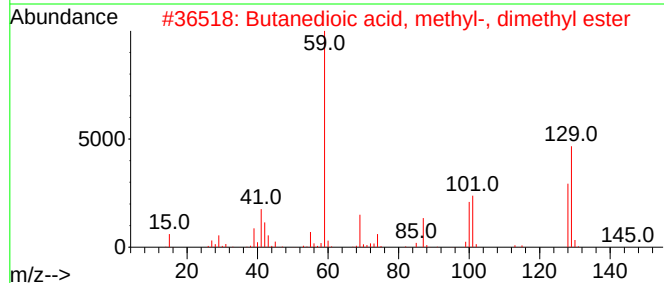
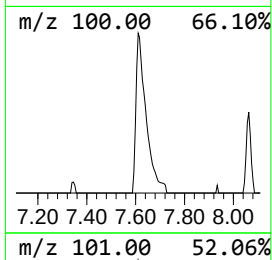
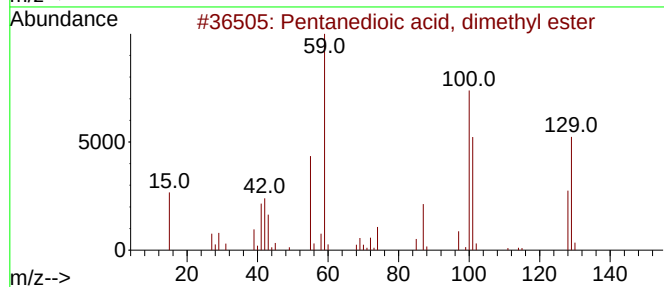
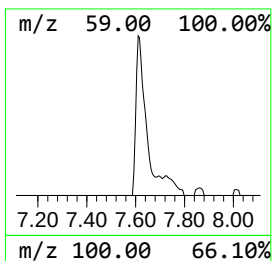
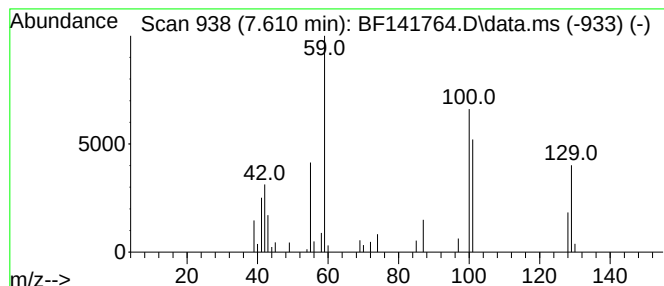
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Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.610	2.23 ng	62196	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	42
3			Hydrazine, trimethyl-	74	C3H10N2	001741-01-1	27
4			Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	27
5			1,4-Di-O-acetyl-2,5-di-O-methyl-...	262	C12H22O6	1000101-82-1	23



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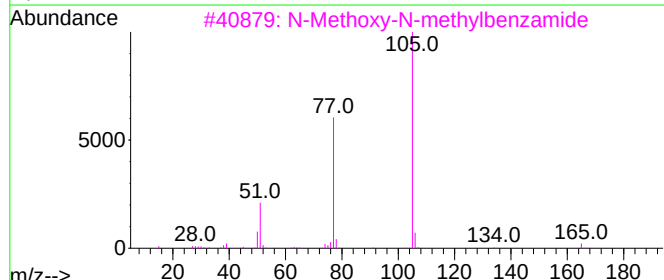
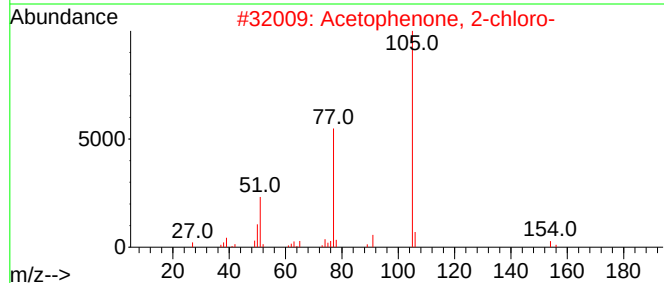
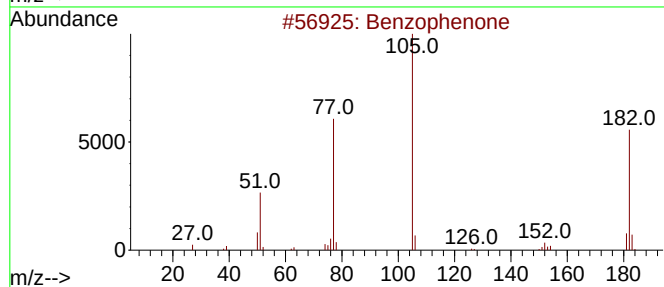
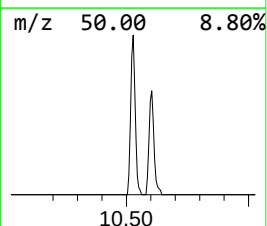
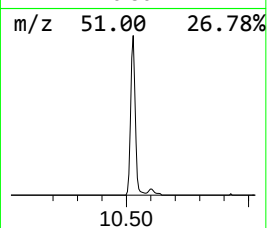
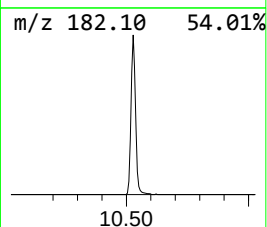
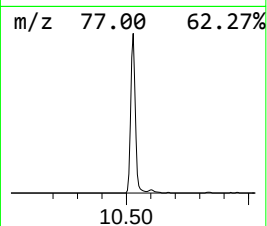
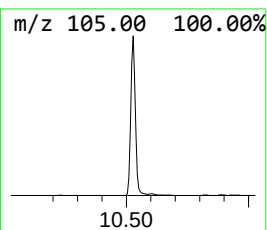
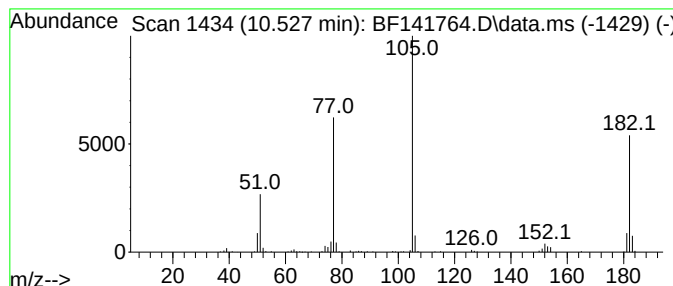
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Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	8.98 ng	278775	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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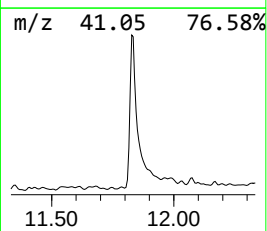
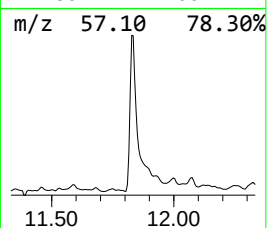
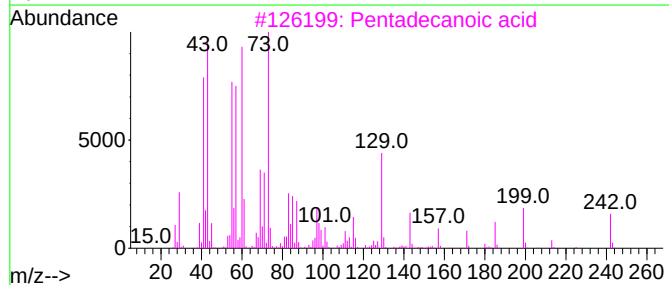
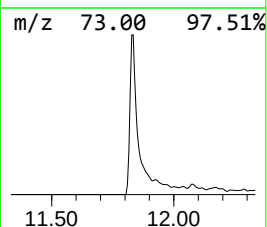
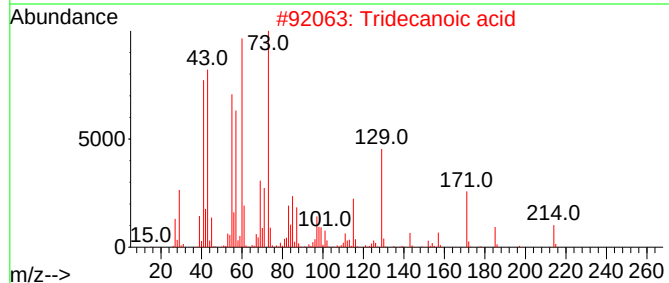
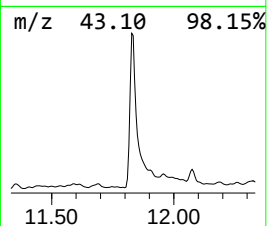
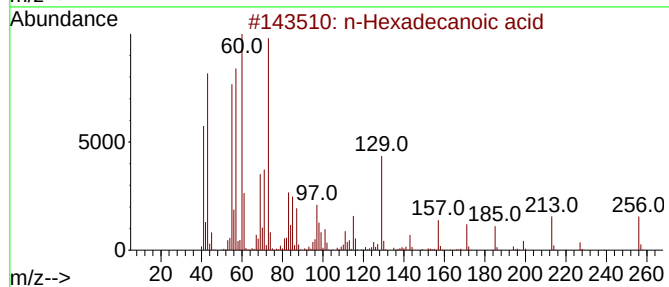
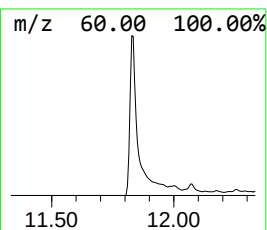
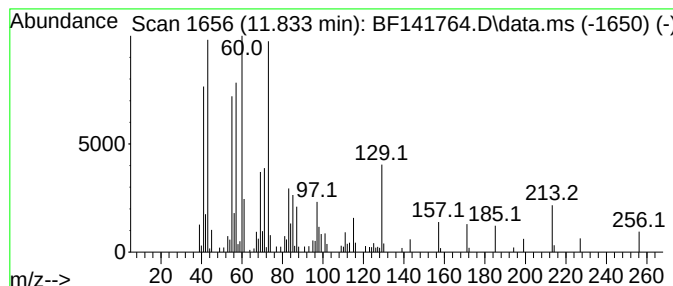
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	7.97 ng	227584	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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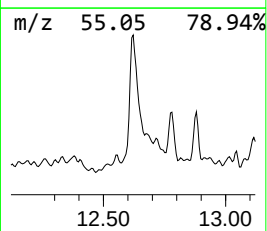
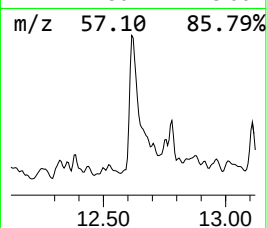
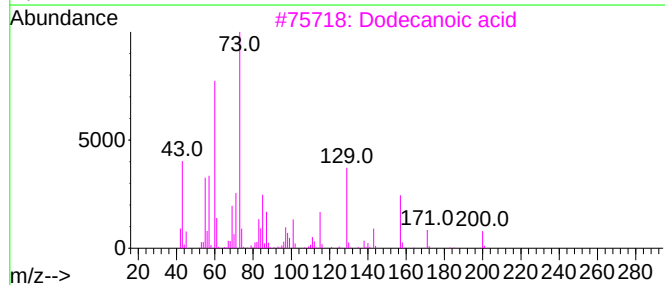
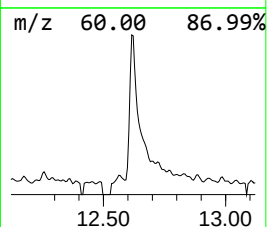
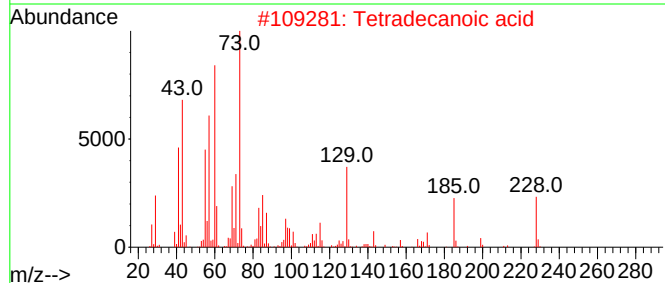
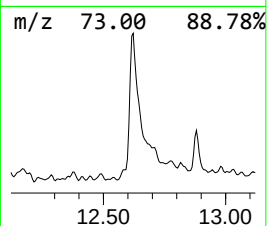
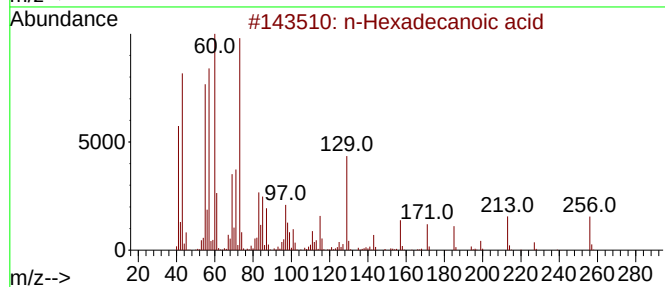
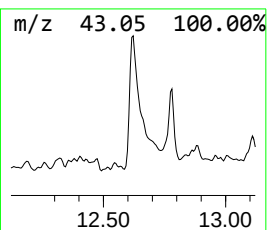
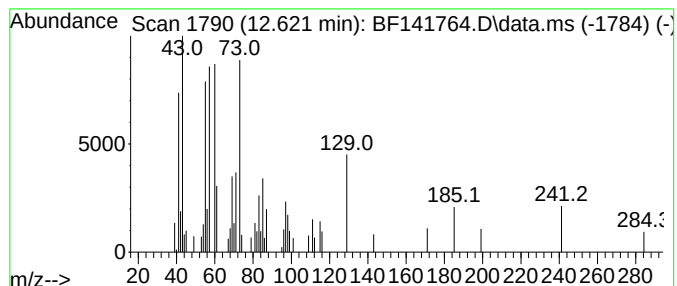
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.621	3.94 ng	85633	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			Dodecanoic acid	200	C12H24O2	000143-07-7	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	52
5			Octadecanoic acid	284	C18H36O2	000057-11-4	49



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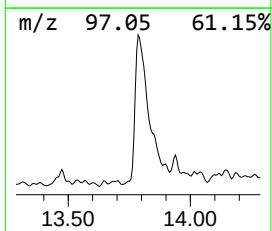
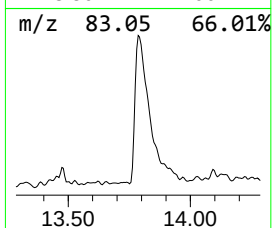
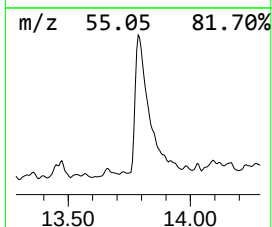
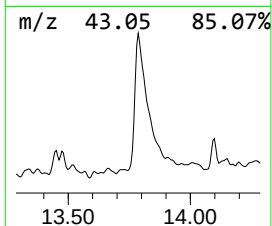
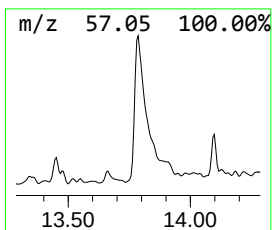
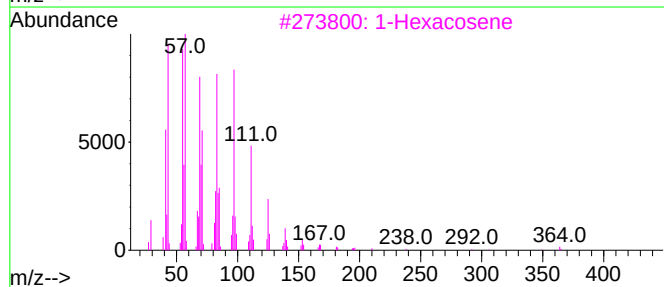
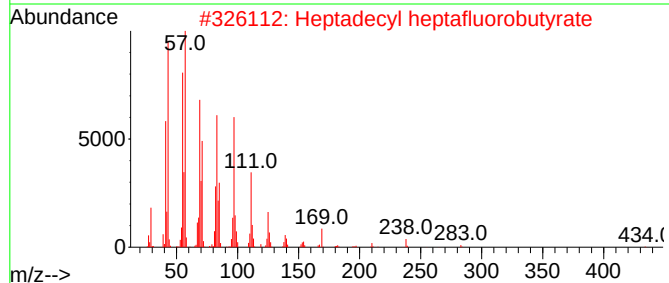
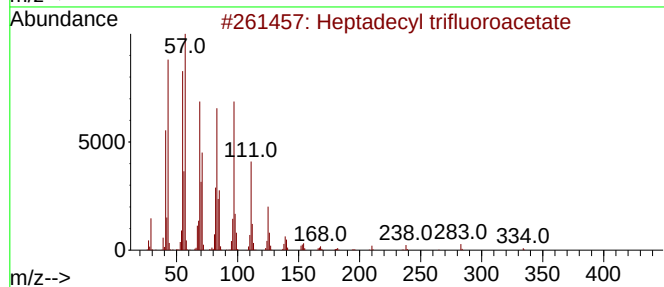
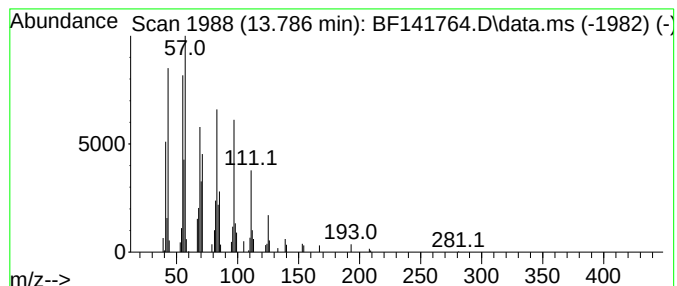
Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF01-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.786	8.15 ng	177187	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	1-Tricosene	322	C23H46	018835-32-0	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141764.D
Acq On : 25 Feb 2025 15:06
Operator : RC/JU
Sample : Q1421-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF01-02

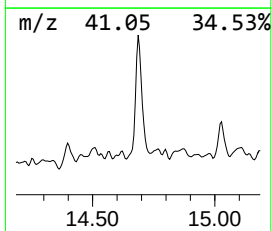
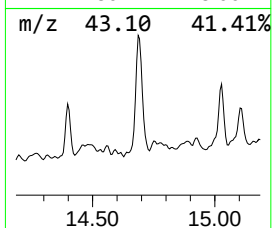
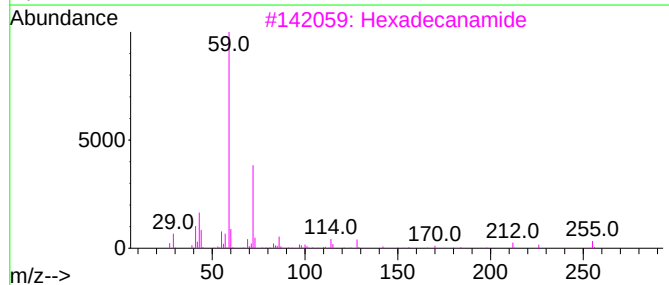
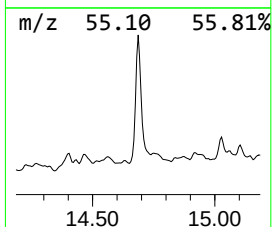
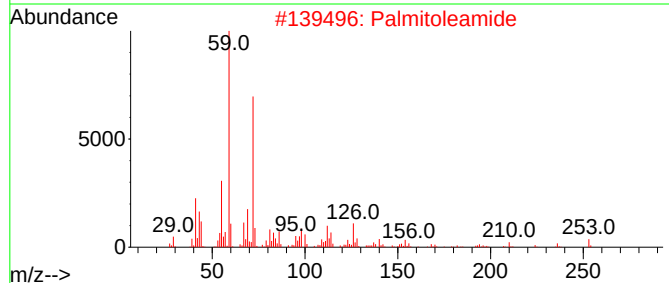
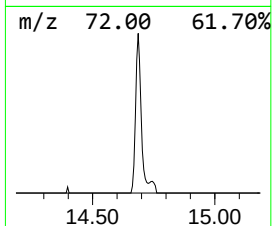
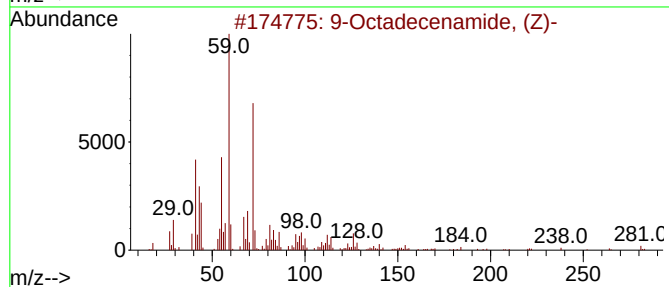
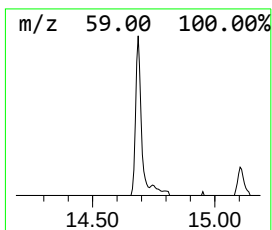
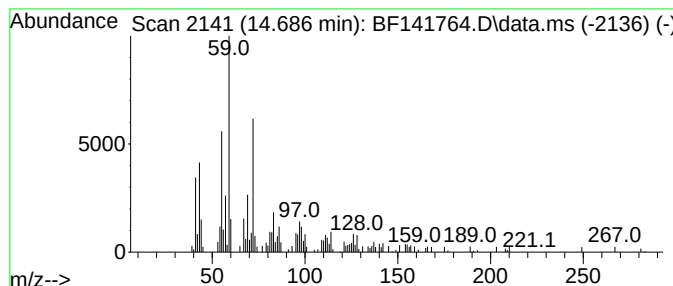
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.686	3.58 ng	83900	Perylene-d12	15.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Palmitoleamide	253	C16H31NO	106010-22-4	80
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
5		2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141764.D
Acq On : 25 Feb 2025 15:06
Operator : RC/JU
Sample : Q1421-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF01-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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-...	4.993	3.1	ng	65834	1	6.781	425207	20.0
Pentanedioic ac...	7.610	2.2	ng	62196	2	8.063	557597	20.0
Benzophenone	10.528	9.0	ng	278775	3	9.816	620550	20.0
n-Hexadecanoic ...	11.833	8.0	ng	227584	4	11.298	571442	20.0
Tetradecanoic acid	12.621	3.9	ng	85633	5	13.939	434778	20.0
Heptadecyl trif...	13.786	8.2	ng	177187	5	13.939	434778	20.0
9-Octadecenamid...	14.686	3.6	ng	83900	6	15.386	469029	20.0