

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081225\
 Data File : BF143355.D
 Acq On : 12 Aug 2025 16:02
 Operator : RC/JU
 Sample : Q2807-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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-BF081225.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	3	9	27	rVB	1232103	1973357	61.73%	7.728%
2	4.057	310	317	326	rVB	26030	39863	1.25%	0.156%
3	5.157	497	504	518	rBV	235554	348910	10.92%	1.366%
4	5.563	567	573	592	rBV	2150646	2813892	88.03%	11.020%
5	6.557	736	742	766	rVB	2099054	2785875	87.15%	10.910%
6	6.928	800	805	812	rBV	733868	901080	28.19%	3.529%
7	7.481	894	899	909	rBV	1374369	1848979	57.84%	7.241%
8	8.210	1017	1023	1040	rBV	880181	1153617	36.09%	4.518%
9	9.280	1199	1205	1210	rBV	2574387	3196544	100.00%	12.519%
10	9.963	1316	1321	1333	rVB	941591	1173020	36.70%	4.594%
11	10.374	1386	1391	1400	rVB	293526	366828	11.48%	1.437%
12	10.669	1436	1441	1449	rBV	299768	396068	12.39%	1.551%
13	10.751	1449	1455	1471	rBV	1264039	1650068	51.62%	6.462%
14	10.980	1486	1494	1500	rBV	61036	88271	2.76%	0.346%
15	11.451	1569	1574	1581	rBV	787358	1046763	32.75%	4.099%
16	11.680	1608	1613	1622	rBV2	40648	92690	2.90%	0.363%
17	11.827	1633	1638	1644	rVB2	76271	110292	3.45%	0.432%
18	11.969	1657	1662	1666	rBV	124412	190349	5.95%	0.745%
19	12.221	1700	1705	1712	rVB2	73946	107829	3.37%	0.422%
20	12.663	1776	1780	1786	rBV	21675	33475	1.05%	0.131%
21	12.757	1791	1796	1804	rBV	38095	75862	2.37%	0.297%
22	12.892	1815	1819	1834	rVB	25768	59863	1.87%	0.234%
23	13.027	1837	1842	1853	rBV	2029008	2730524	85.42%	10.693%
24	13.933	1991	1996	2007	rBV	78154	163426	5.11%	0.640%
25	14.086	2016	2022	2034	rBV	689554	947253	29.63%	3.710%
26	14.839	2146	2150	2159	rBV2	94340	188662	5.90%	0.739%
27	15.574	2270	2275	2287	rVB	656241	1051096	32.88%	4.116%

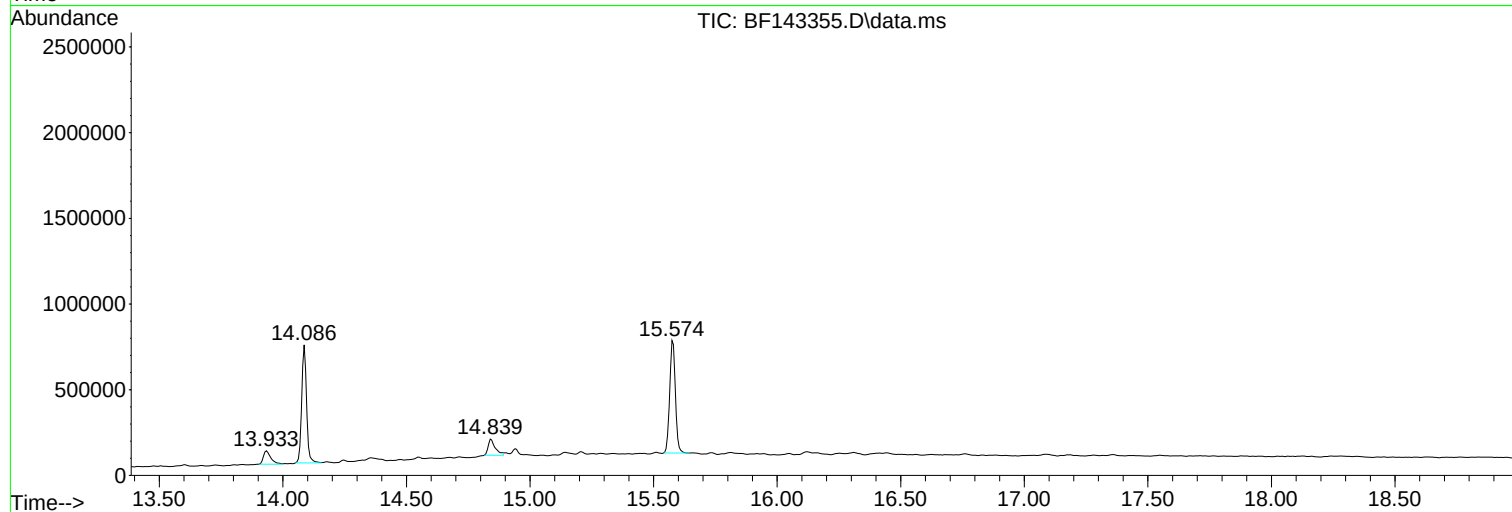
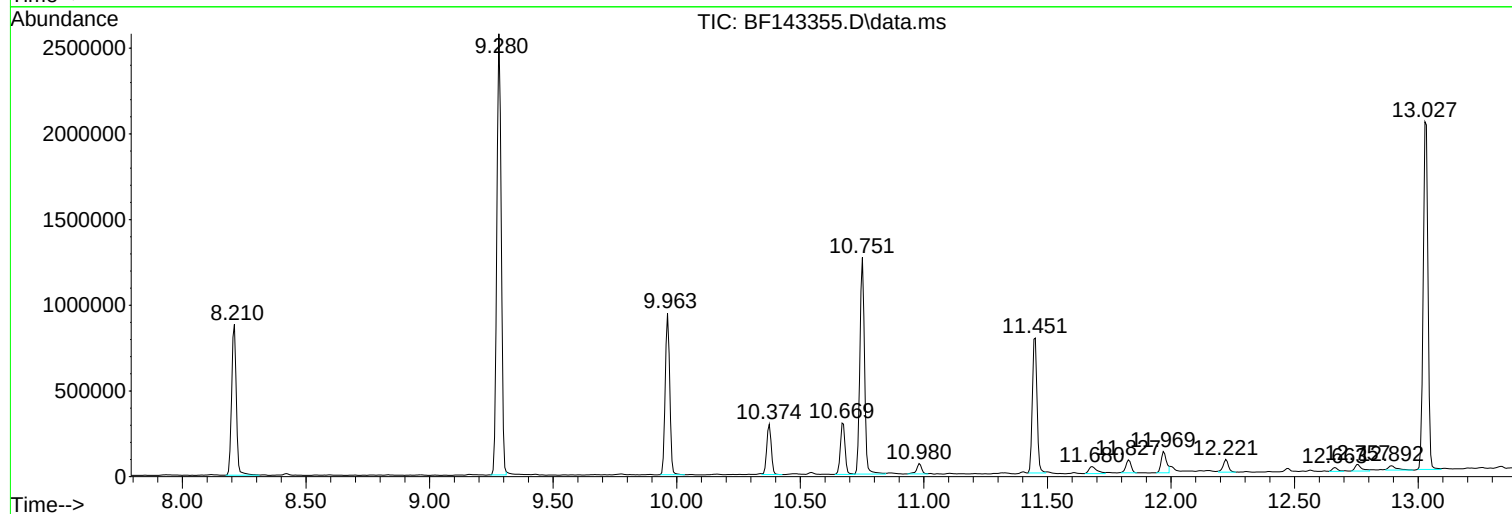
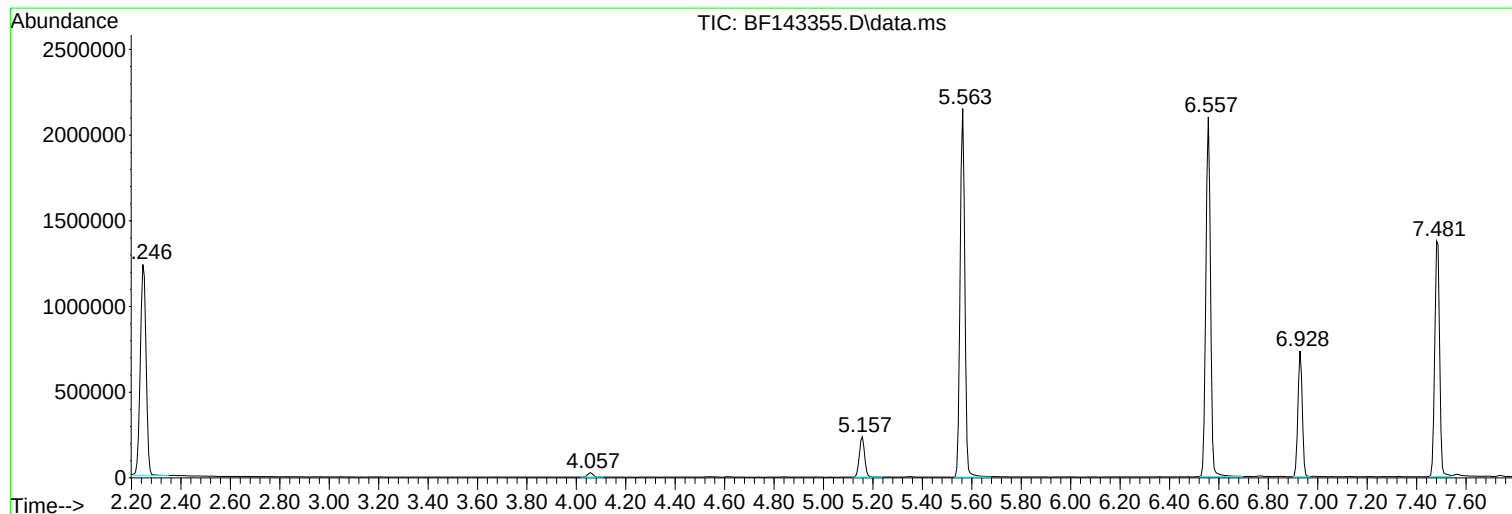
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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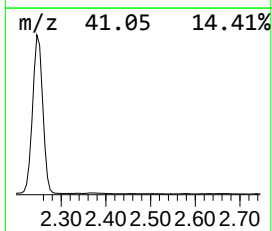
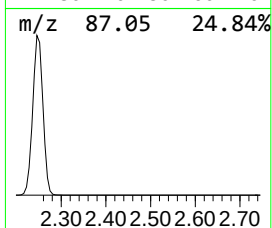
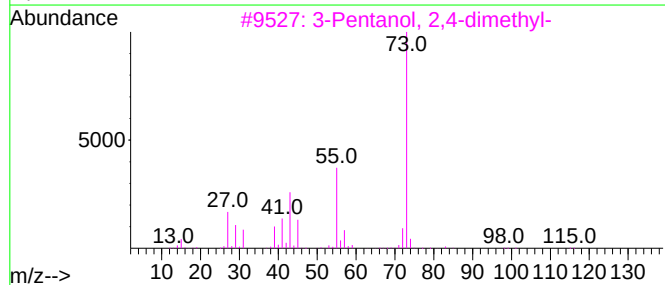
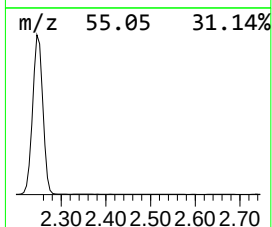
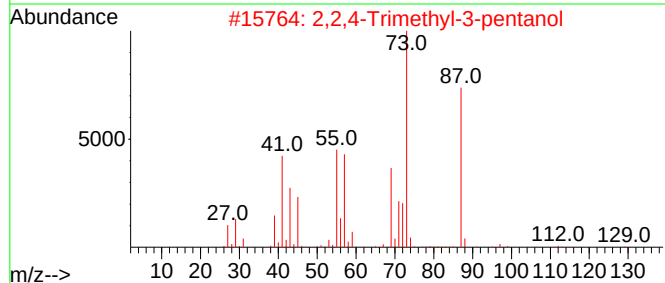
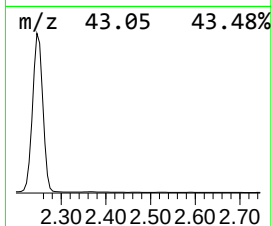
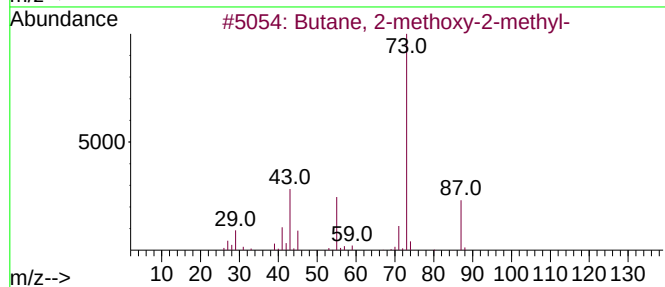
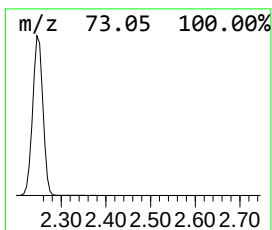
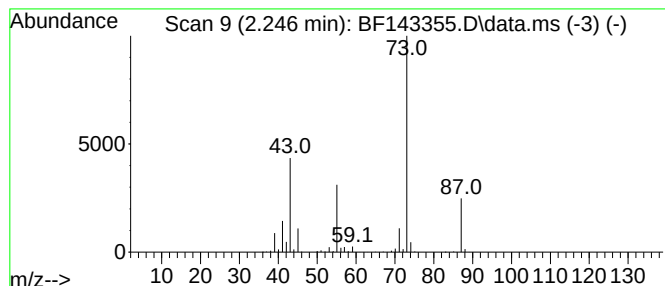
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	43.80 ng	1973360	1,4-Dichlorobenzene-d4	6.928

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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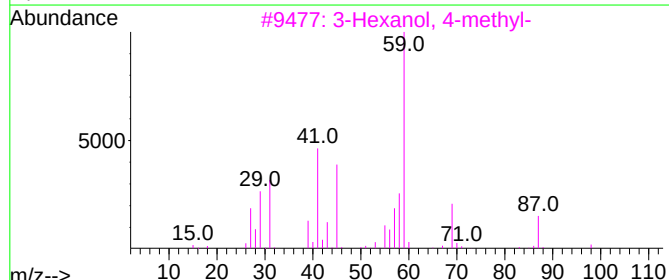
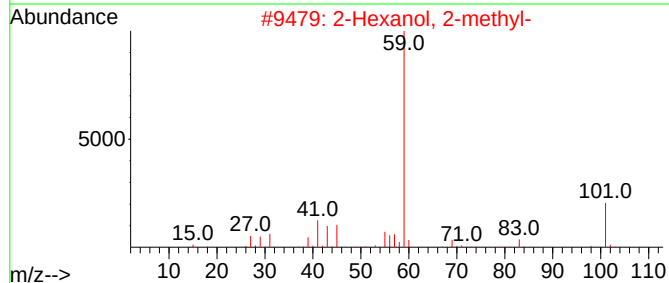
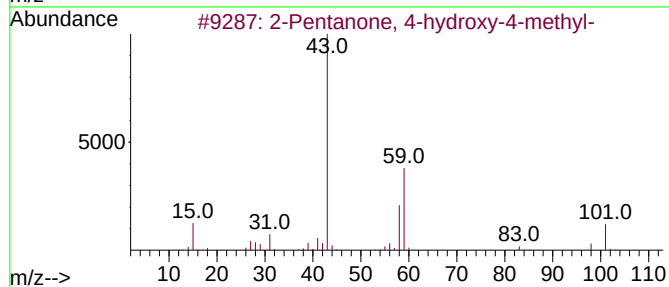
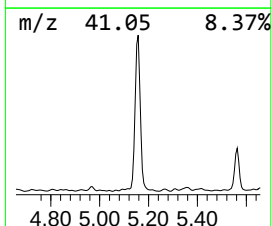
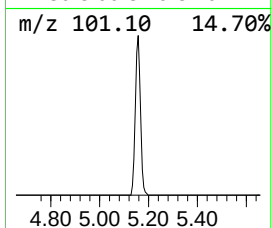
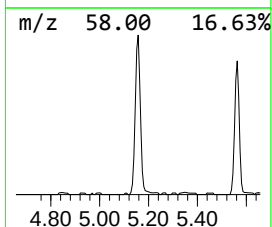
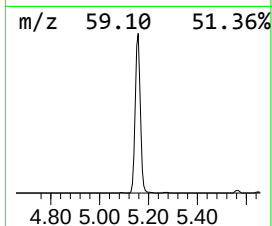
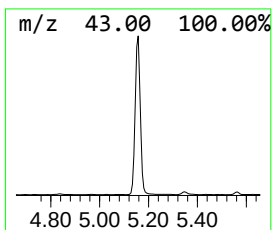
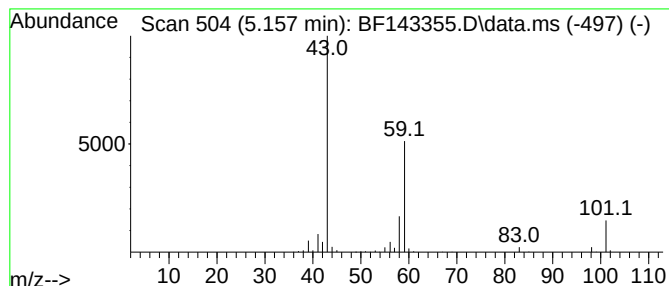
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	7.74 ng	348910	1,4-Dichlorobenzene-d4	6.928

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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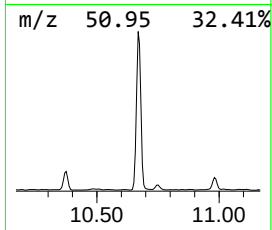
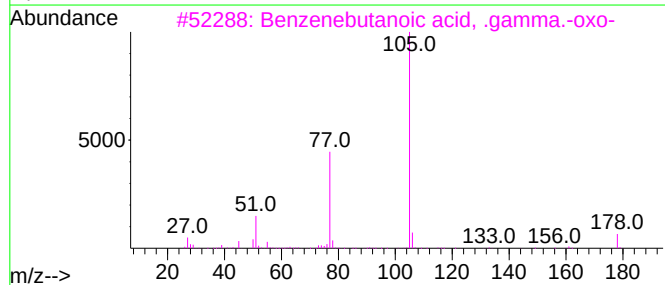
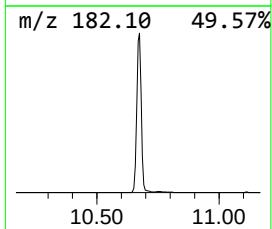
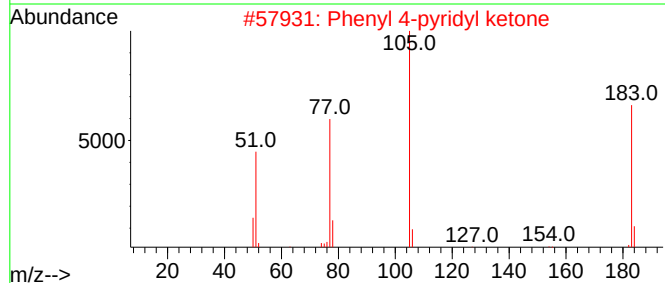
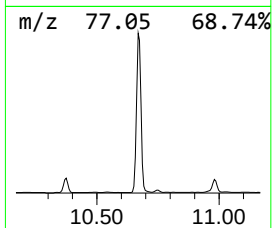
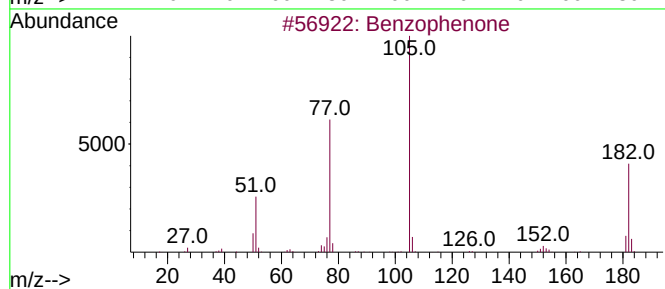
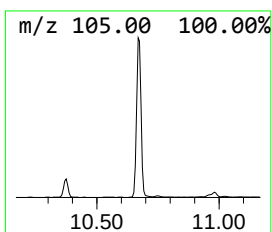
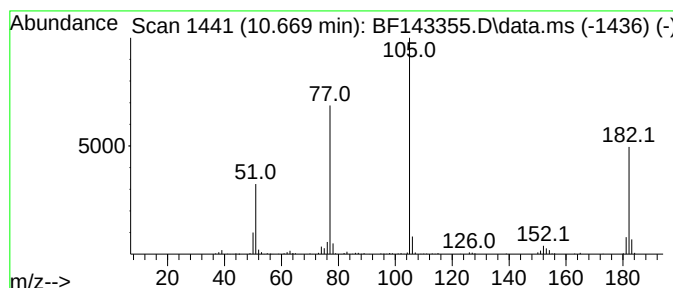
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.669	6.75 ng	396068	Acenaphthene-d10	9.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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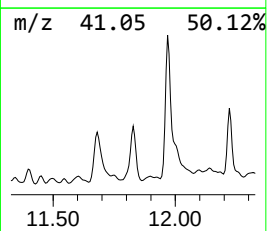
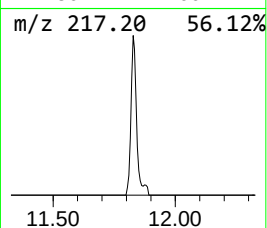
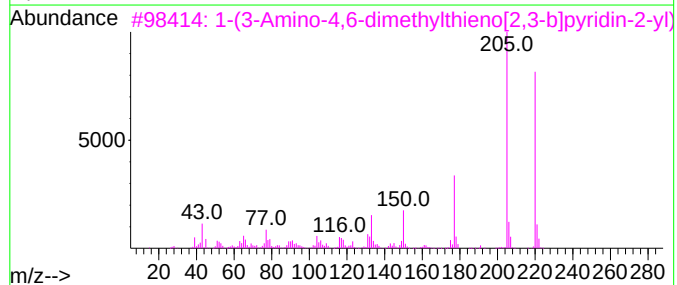
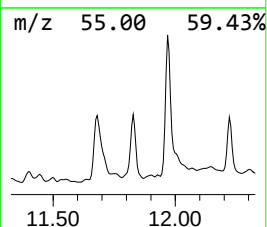
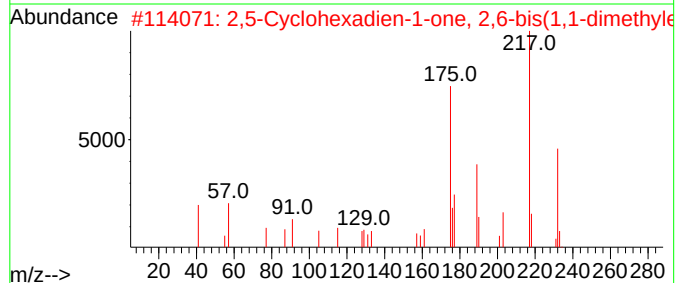
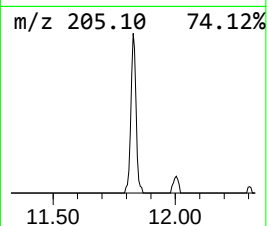
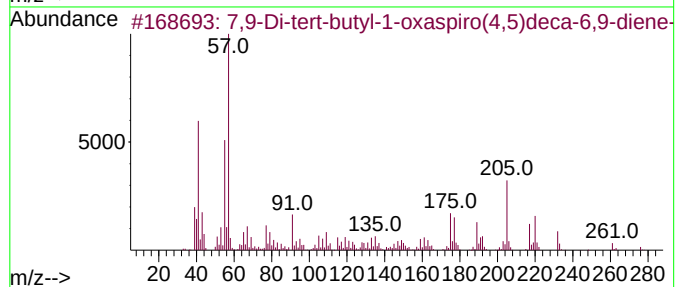
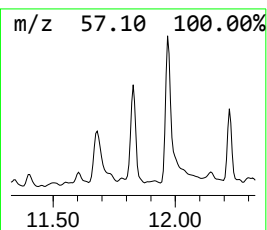
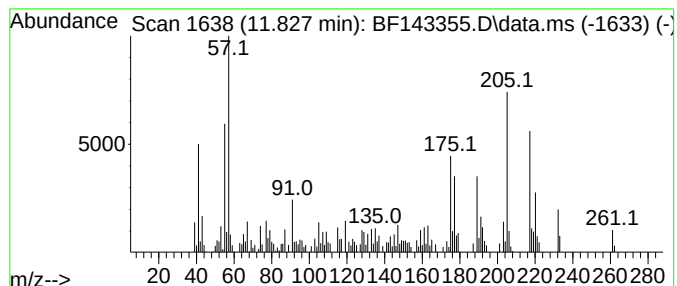
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.827	2.11 ng	110292	Phenanthrene-d10		11.451	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	87
2	2,5-Cyclohexadien-1-one, 2,6-bis...		232	C16H24O	006738-27-8	52
3	1-(3-Amino-4,6-dimethylthieno[2,...		220	C11H12N2OS	052505-42-7	50
4	2,6-Bis(1,1-dimethylethyl)-4-met...		262	C18H30O	004278-82-4	42
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...		220	C15H24O	104188-25-2	41



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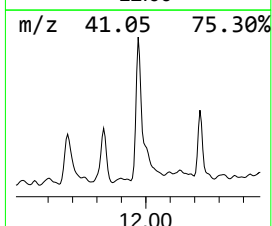
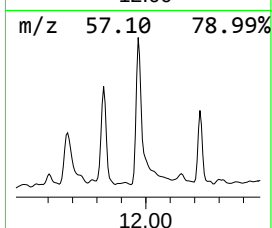
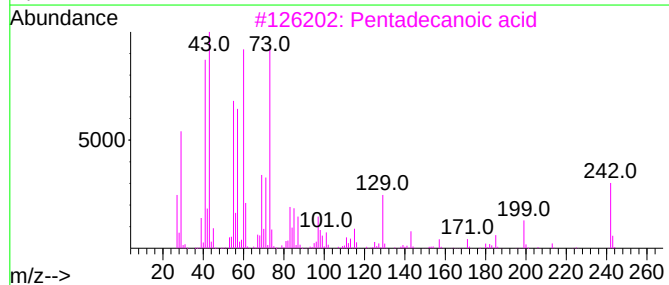
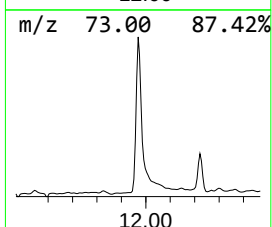
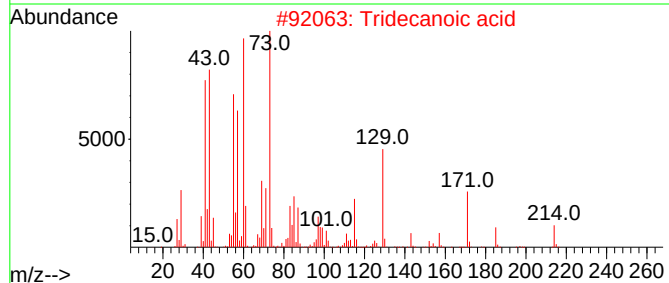
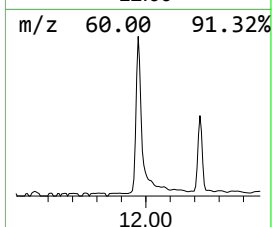
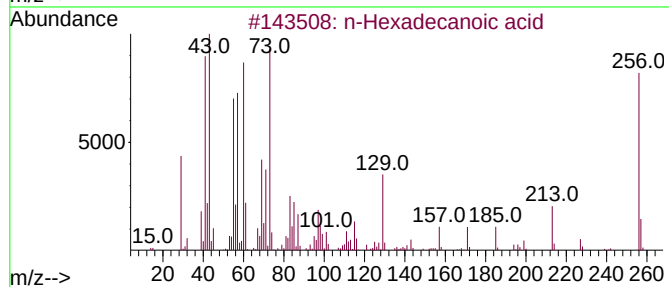
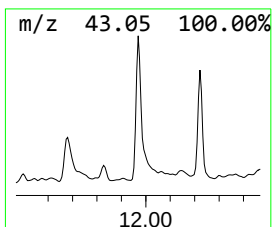
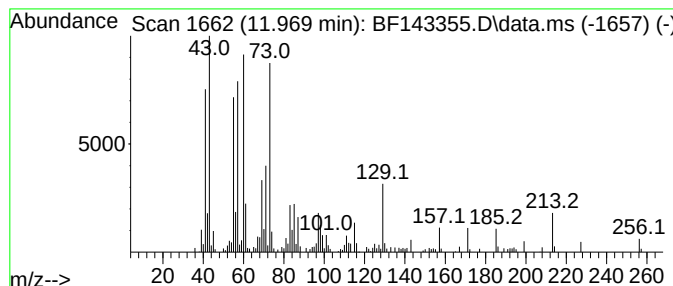
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	3.64 ng	190349	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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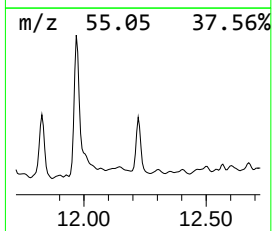
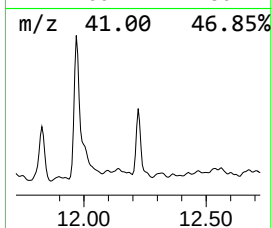
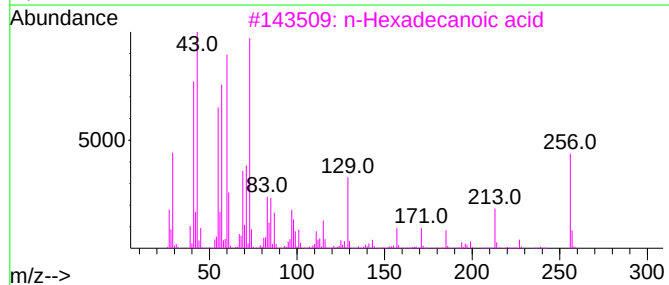
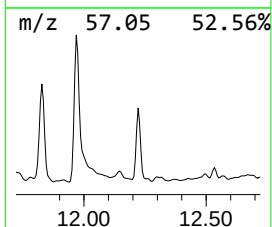
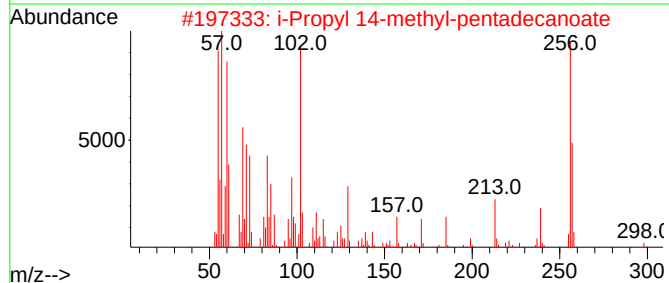
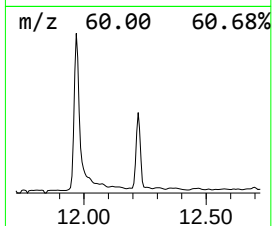
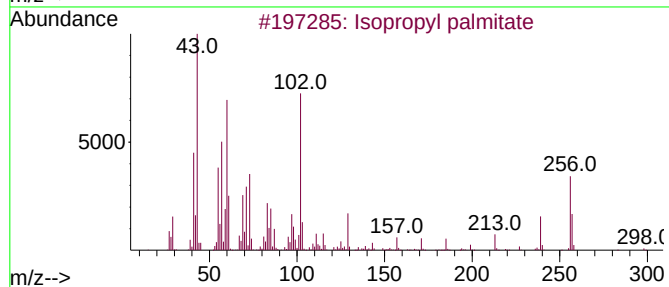
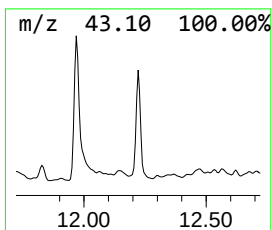
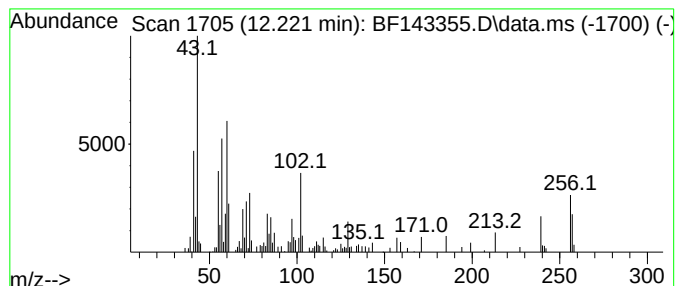
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.221	2.06 ng	107829	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	90
2			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	80
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081225\
Data File : BF143355.D
Acq On : 12 Aug 2025 16:02
Operator : RC/JU
Sample : Q2807-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

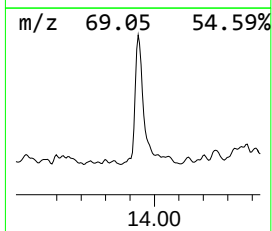
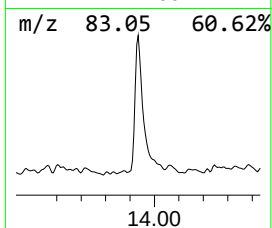
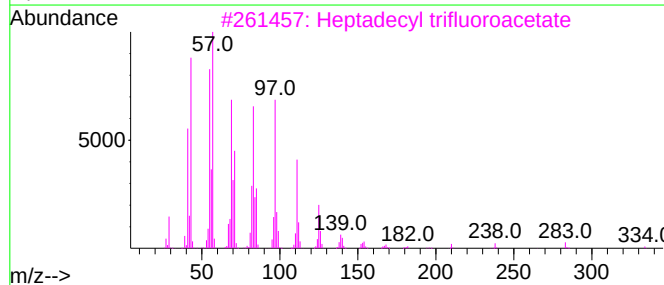
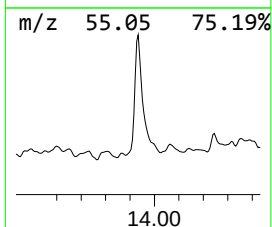
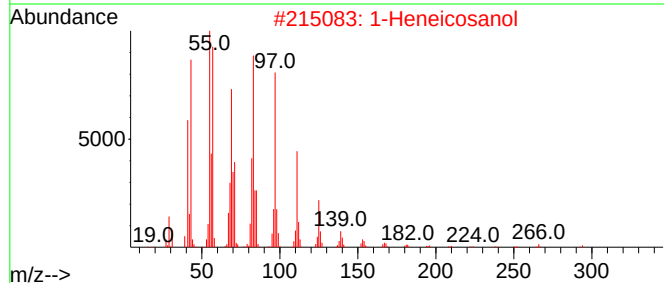
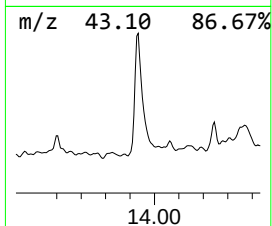
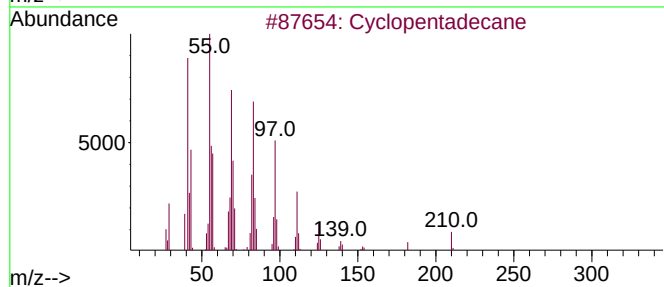
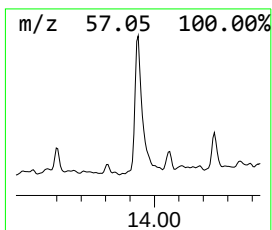
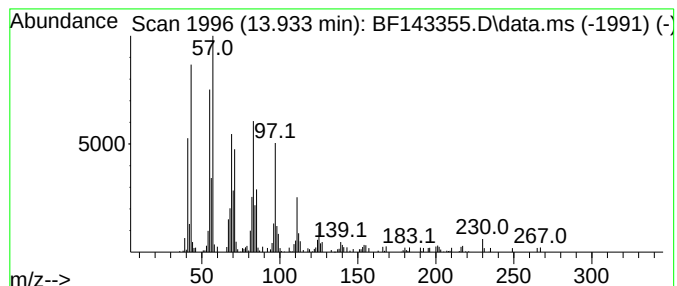
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	3.45 ng	163426	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081225\
Data File : BF143355.D
Acq On : 12 Aug 2025 16:02
Operator : RC/JU
Sample : Q2807-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

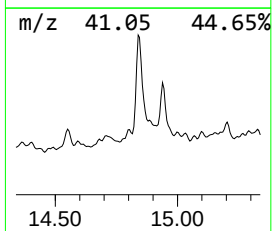
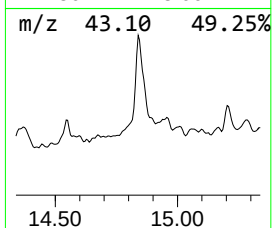
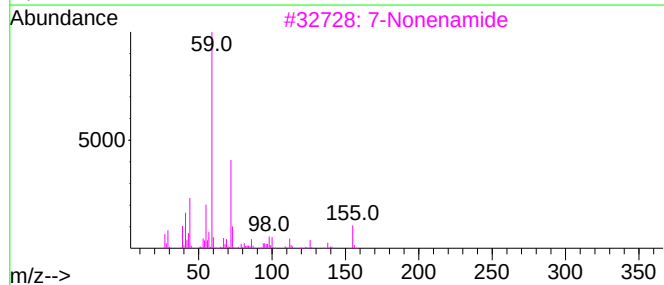
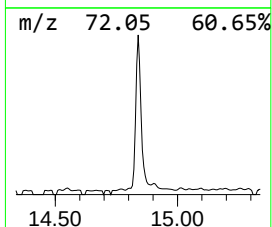
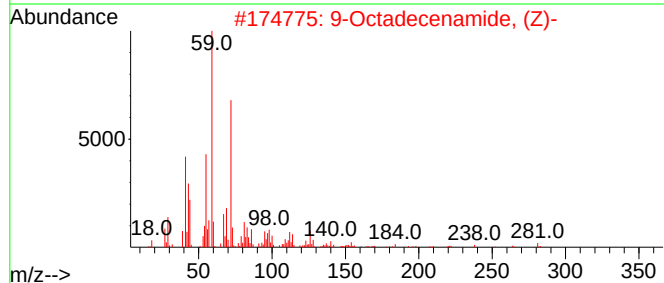
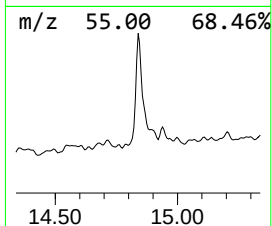
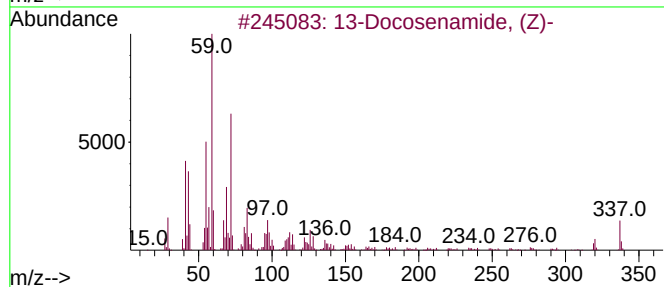
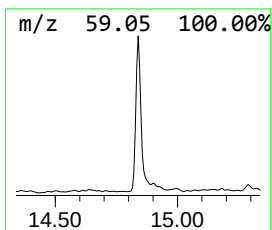
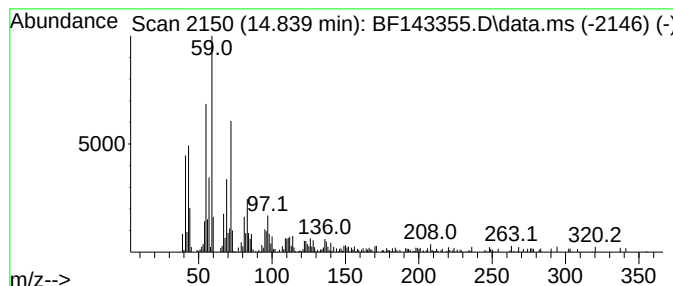
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.839	3.59 ng	188662	Perylene-d12	15.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3	7-Nonenamide	155	C9H17NO	090949-53-4	50
4	Octadecanamide	283	C18H37NO	000124-26-5	49
5	Dodecanamide	199	C12H25NO	001120-16-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081225\
Data File : BF143355.D
Acq On : 12 Aug 2025 16:02
Operator : RC/JU
Sample : Q2807-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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...	2.246	43.8	ng	1973360	1	6.928	901080	20.0
2-Pentanone, 4-...	5.157	7.7	ng	348910	1	6.928	901080	20.0
Benzophenone	10.669	6.8	ng	396068	3	9.963	1173020	20.0
7,9-Di-tert-but...	11.827	2.1	ng	110292	4	11.451	1046760	20.0
n-Hexadecanoic ...	11.969	3.6	ng	190349	4	11.451	1046760	20.0
Isopropyl palmi...	12.221	2.1	ng	107829	4	11.451	1046760	20.0
Cyclopentadecane	13.933	3.5	ng	163426	5	14.086	947253	20.0
13-Docosenamide...	14.839	3.6	ng	188662	6	15.574	1051100	20.0