

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
 Data File : BF132226.D
 Acq On : 30 Jan 2023 23:31
 Operator : CG\JU
 Sample : 01328-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1-BORING-1-0-7

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-BF012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.331	418	424	435	rVB	1590935	2107703	33.79%	5.001%
2	5.707	483	488	491	rBV	4605086	5061536	81.14%	12.009%
3	6.695	650	656	659	rBV	4426423	5040360	80.80%	11.959%
4	7.078	718	721	725	rVB	1483620	1166512	18.70%	2.768%
5	7.642	812	817	820	rBV	3481795	3406507	54.61%	8.082%
6	8.366	936	940	943	rBV	2032483	1548410	24.82%	3.674%
7	9.442	1119	1123	1126	rBV	6849873	6238207	100.00%	14.800%
8	10.130	1236	1240	1243	rBV	2140692	1676685	26.88%	3.978%
9	10.842	1358	1361	1365	rVB	304656	237361	3.80%	0.563%
10	10.925	1370	1375	1378	rBV	3809633	3341844	53.57%	7.929%
11	11.624	1491	1494	1497	rBV	1626265	1439197	23.07%	3.415%
12	12.136	1577	1581	1590	rBV	289520	314810	5.05%	0.747%
13	12.701	1671	1677	1682	rBV5	65565	120259	1.93%	0.285%
14	12.848	1697	1702	1704	rBV	80524	90809	1.46%	0.215%
15	12.924	1712	1715	1722	rBV3	92086	108793	1.74%	0.258%
16	13.024	1729	1732	1734	rVB	69556	67335	1.08%	0.160%
17	13.077	1738	1741	1748	rVV2	85399	120249	1.93%	0.285%
18	13.219	1761	1765	1769	rBV	4979842	4751066	76.16%	11.272%
19	13.436	1799	1802	1804	rBV	80675	66546	1.07%	0.158%
20	13.783	1858	1861	1868	rBV2	81198	100973	1.62%	0.240%
21	14.113	1914	1917	1919	rBV	102720	106059	1.70%	0.252%
22	14.289	1943	1947	1950	rBV	1247450	1111373	17.82%	2.637%
23	14.430	1968	1971	1976	rBV	134252	142616	2.29%	0.338%
24	14.748	2022	2025	2029	rVB	108502	106689	1.71%	0.253%
25	14.924	2051	2055	2063	rBV	2170224	2123996	34.05%	5.039%
26	15.083	2080	2082	2086	rVB	110992	108040	1.73%	0.256%
27	15.465	2143	2147	2151	rBV	119030	145813	2.34%	0.346%
28	15.877	2213	2217	2226	rVB2	742797	1112261	17.83%	2.639%
29	16.677	2350	2353	2364	rVB3	90995	186665	2.99%	0.443%

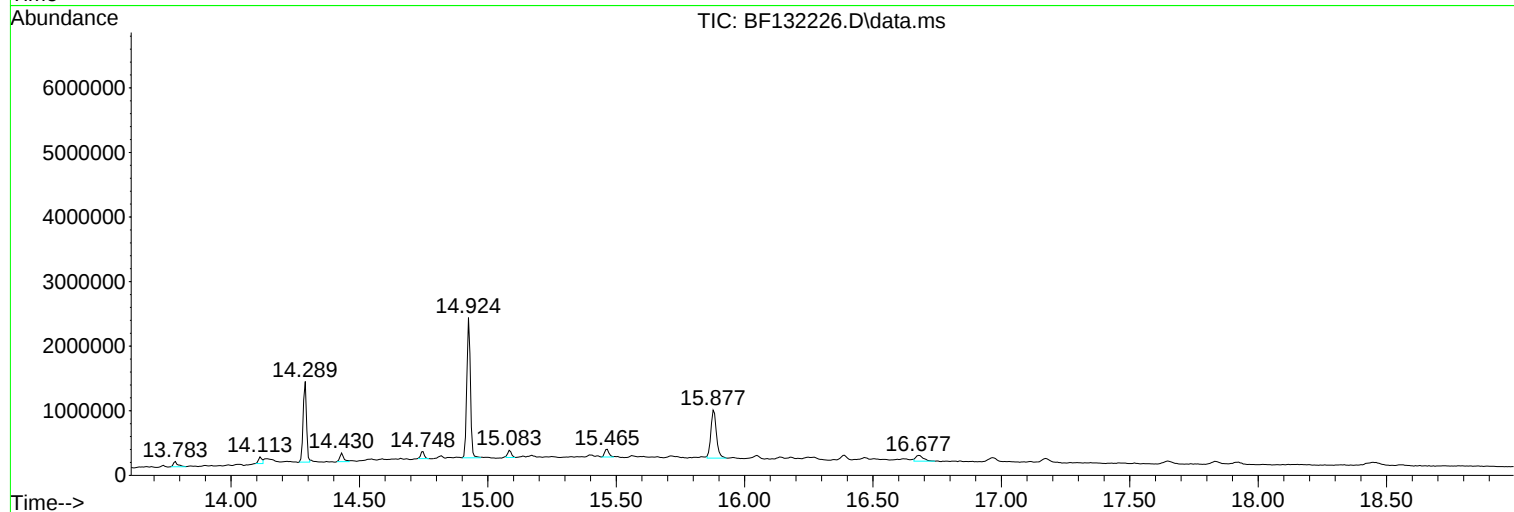
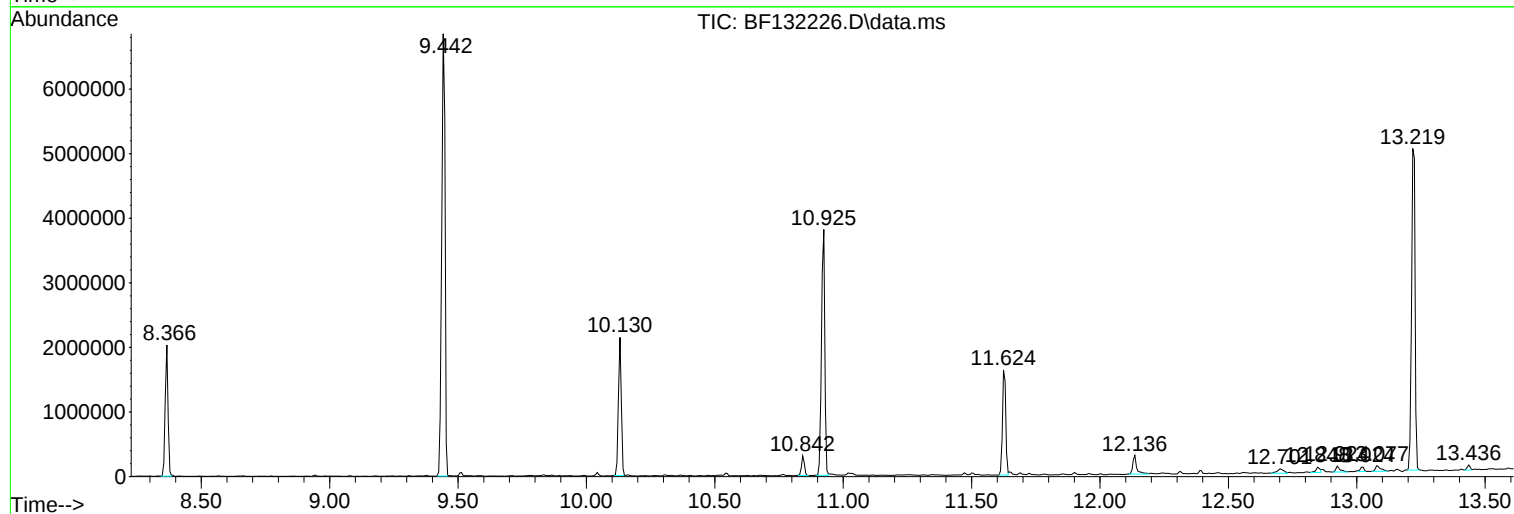
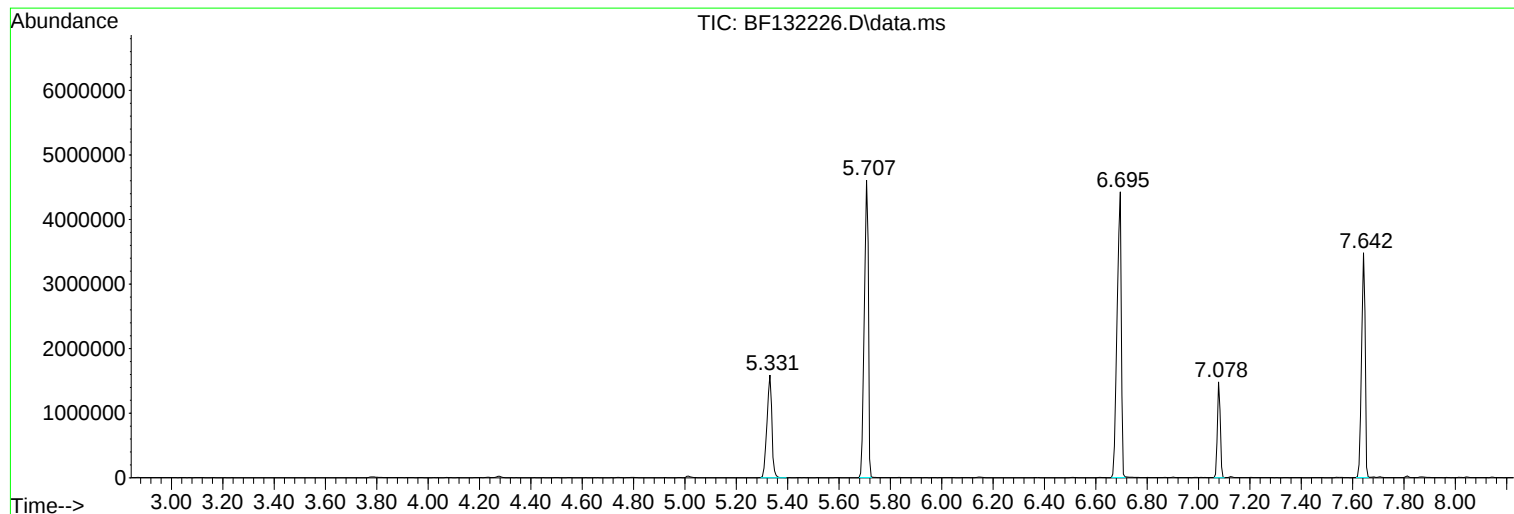
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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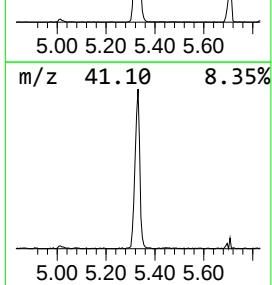
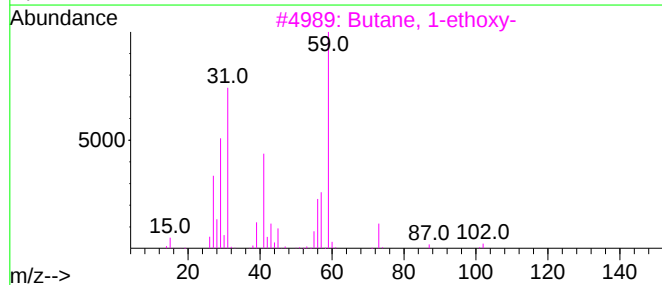
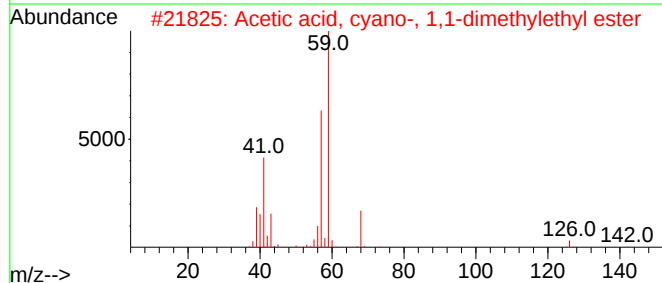
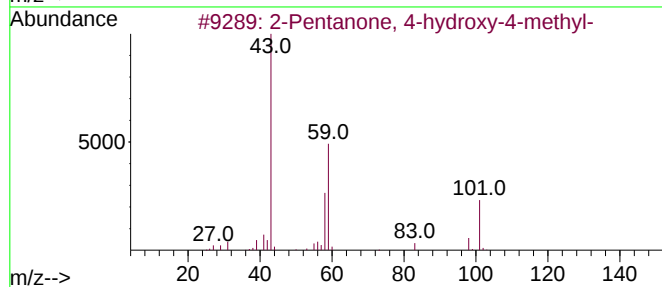
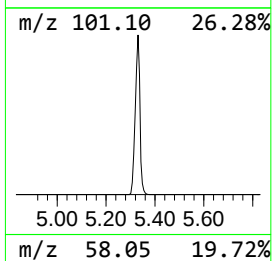
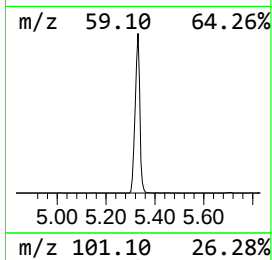
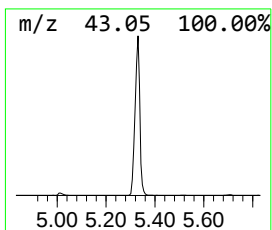
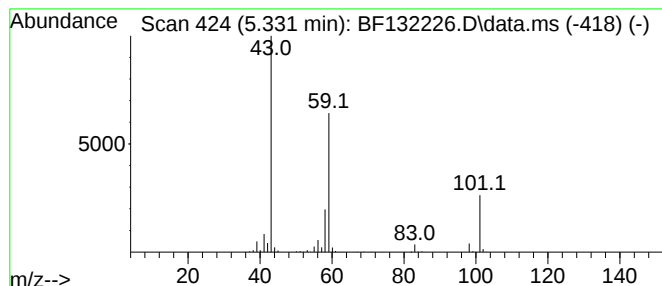
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.331	36.14 ng	2107700	1,4-Dichlorobenzene-d4	7.078

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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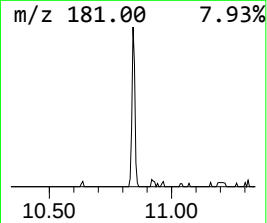
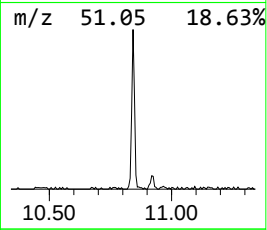
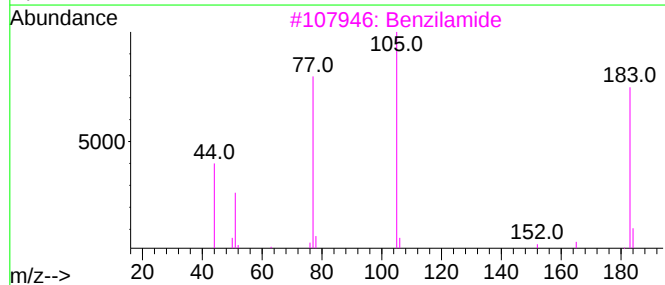
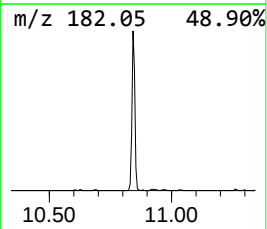
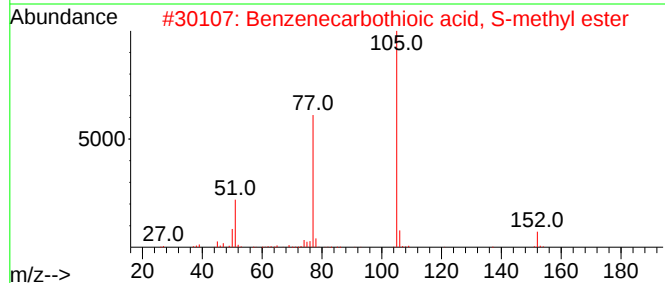
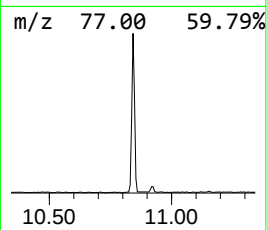
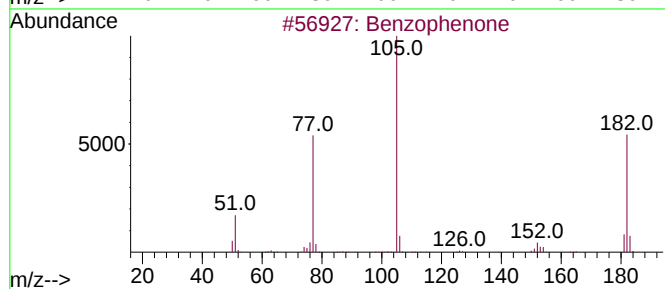
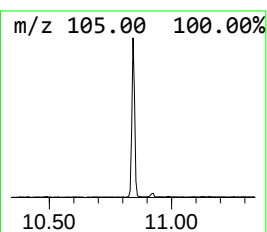
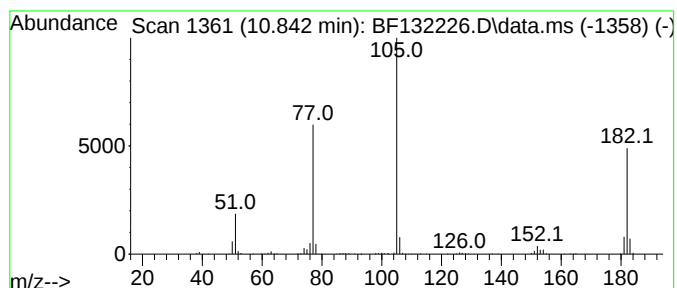
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.842	2.83 ng	237361	Acenaphthene-d10	10.131

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Benzilamide	227	C14H13NO2	004746-87-6	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43



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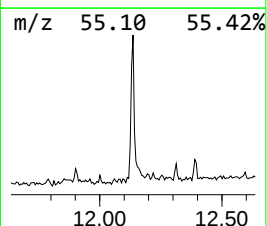
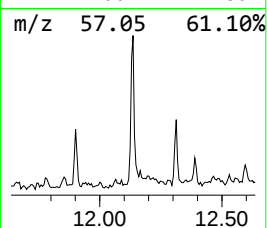
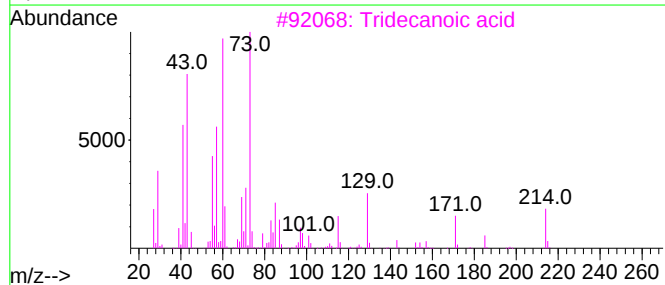
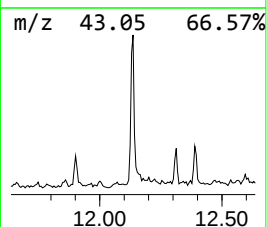
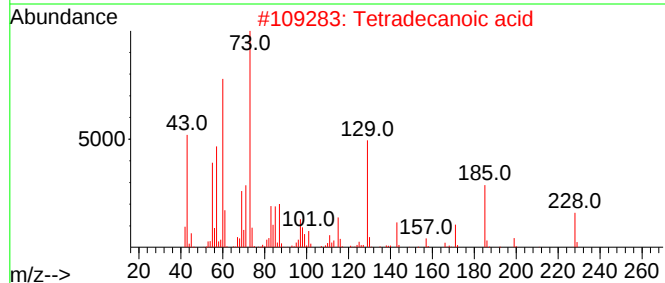
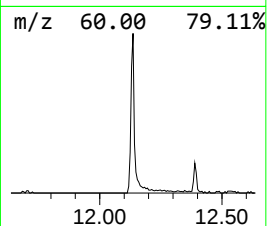
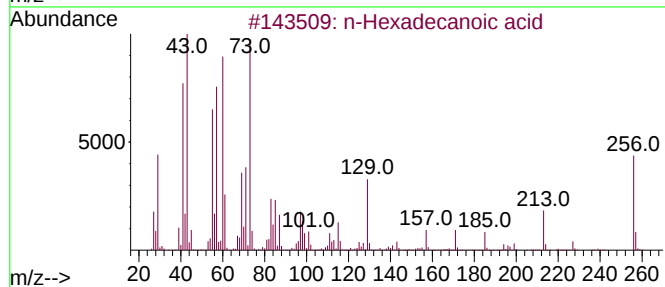
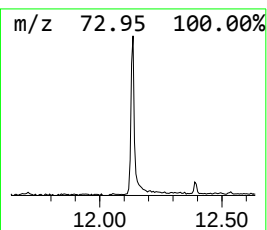
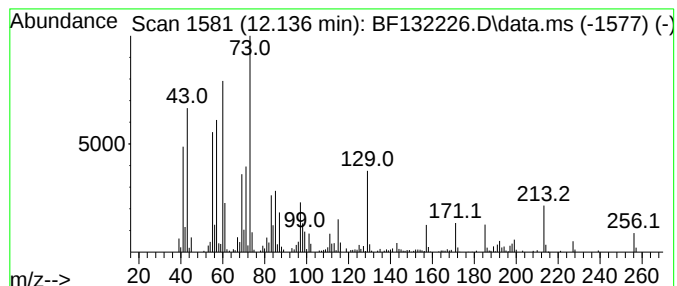
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.136	4.37 ng	314810	Phenanthrene-d10	11.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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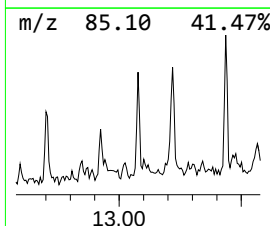
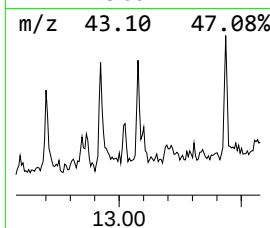
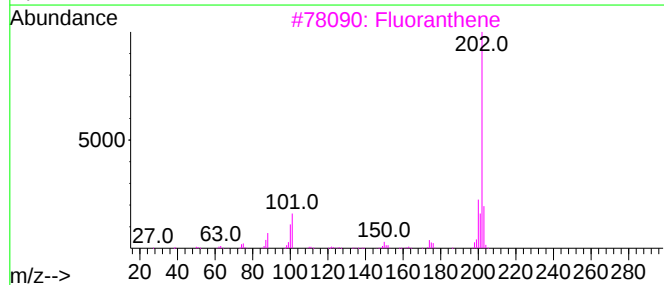
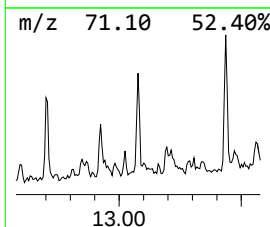
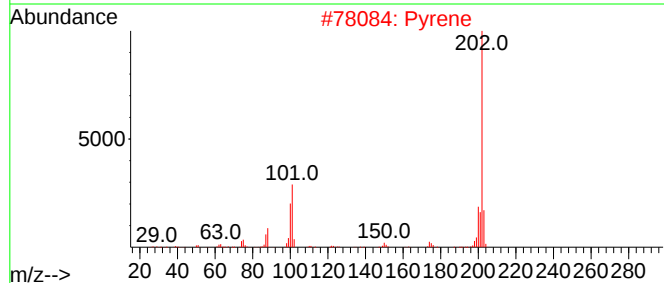
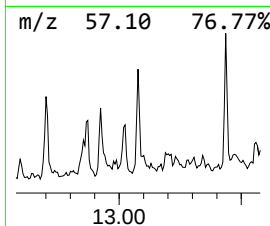
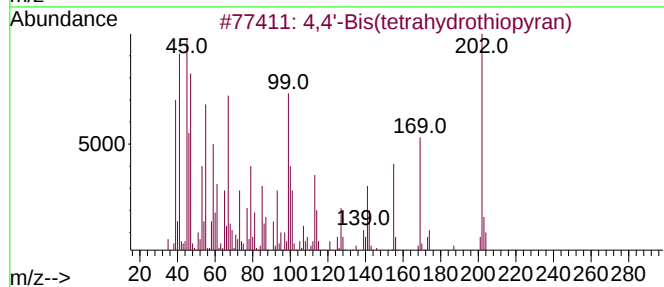
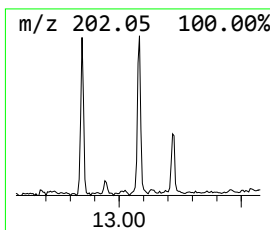
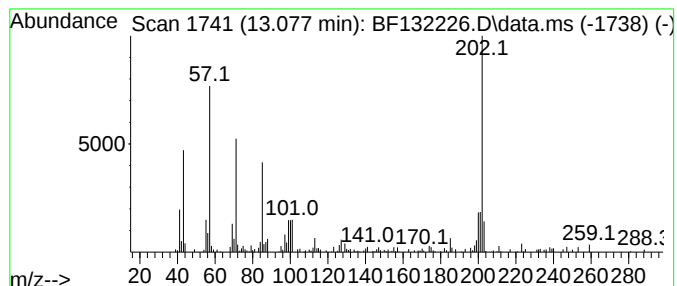
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.077	2.16 ng	120249	Chrysene-d12	14.289

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	95
2		Pyrene	202	C16H10	000129-00-0	50
3		Fluoranthene	202	C16H10	000206-44-0	50
4		Heptadecane	240	C17H36	000629-78-7	47
5		Heneicosane	296	C21H44	000629-94-7	41



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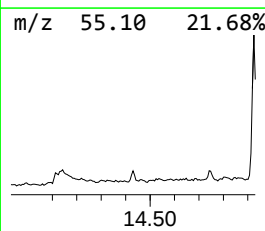
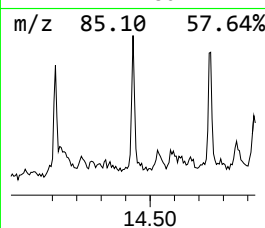
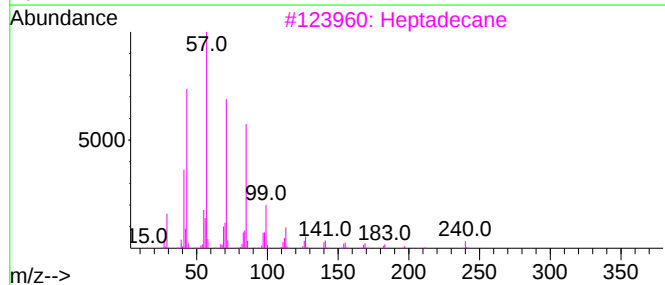
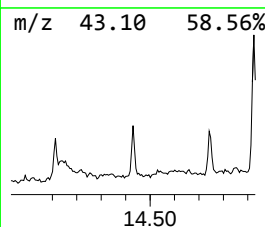
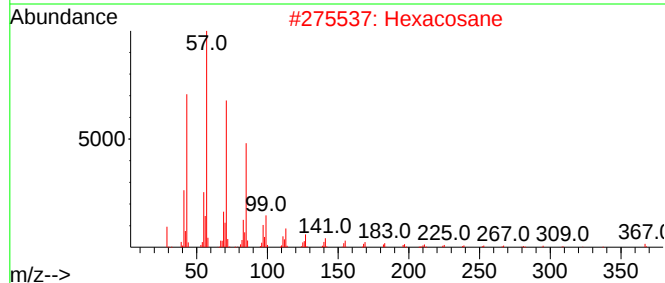
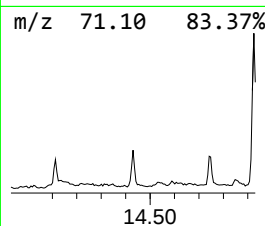
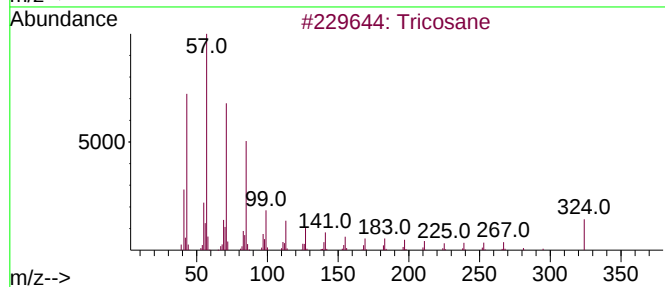
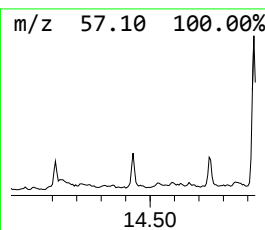
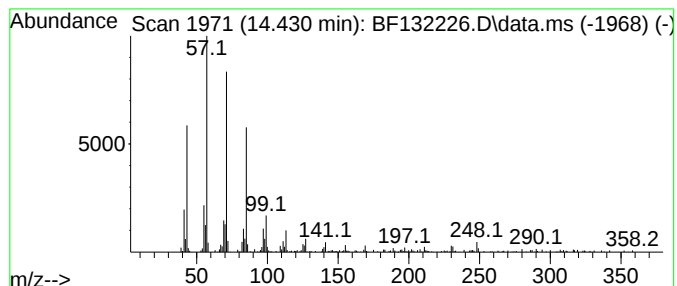
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Peak Number 5 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.430	2.57 ng	142616	Chrysene-d12	14.289

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	93
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heptadecane	240	C17H36	000629-78-7	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Octacosane	394	C28H58	000630-02-4	87



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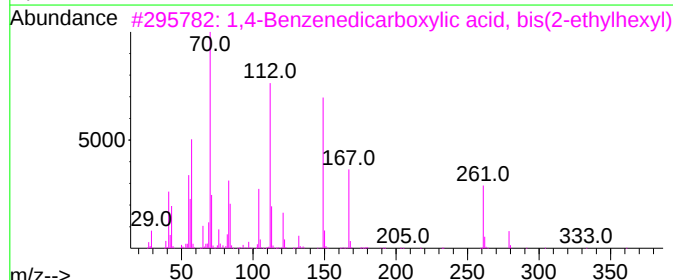
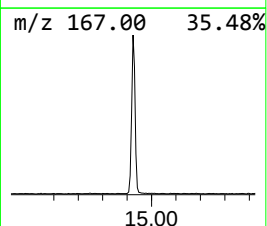
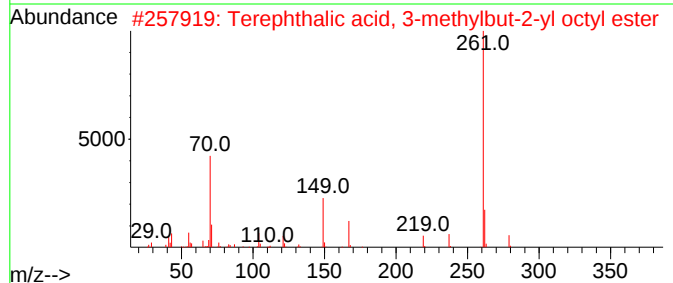
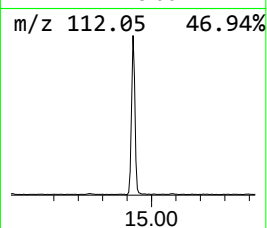
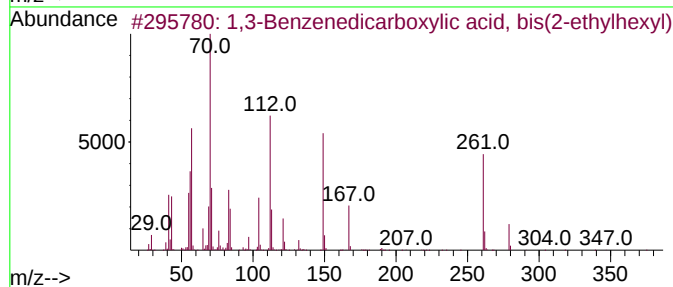
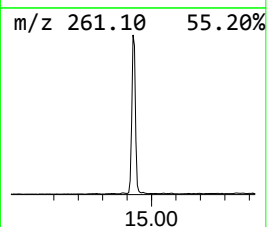
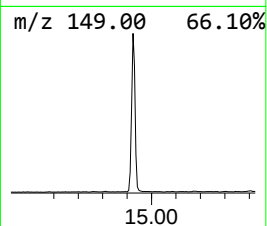
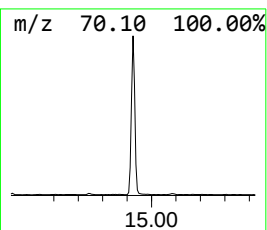
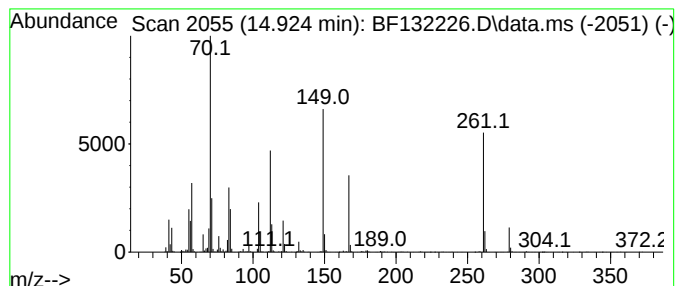
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.924	38.22 ng	2124000	Chrysene-d12	14.289

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
3			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
4			Isophthalic acid, 3-methylbut-2...	348	C21H32O4	1000344-72-4	50
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
Data File : BF132226.D
Acq On : 30 Jan 2023 23:31
Operator : CG\JU
Sample : 01328-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-BORING-1-0-7

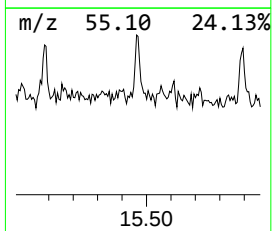
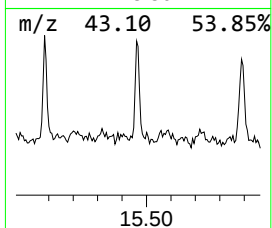
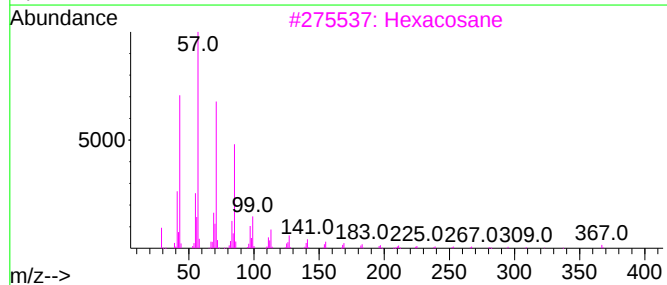
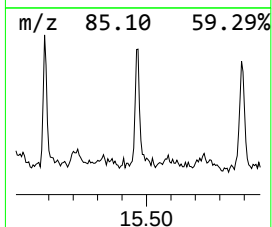
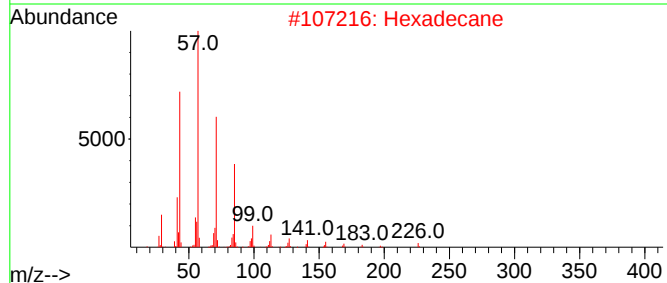
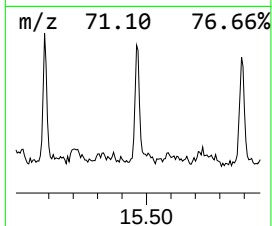
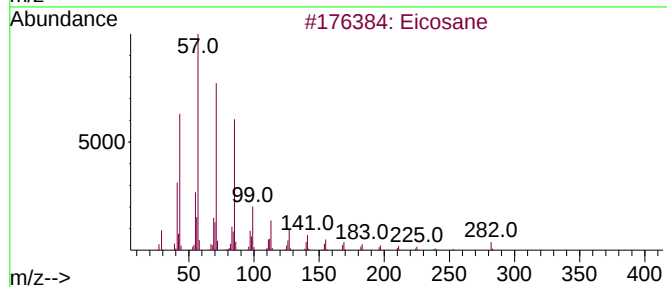
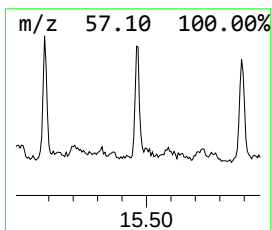
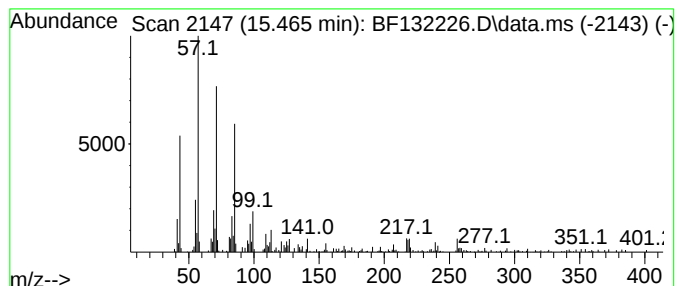
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.465	2.62 ng	145813	Perylene-d12	15.877

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Hexadecane	226	C16H34	000544-76-3	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			2-Methyltetracosane	352	C25H52	001560-78-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
Data File : BF132226.D
Acq On : 30 Jan 2023 23:31
Operator : CG\JU
Sample : 01328-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-BORING-1-0-7

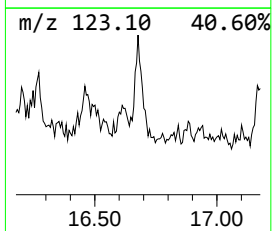
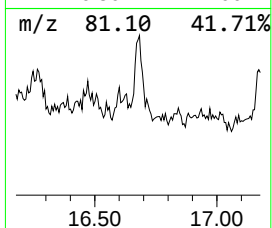
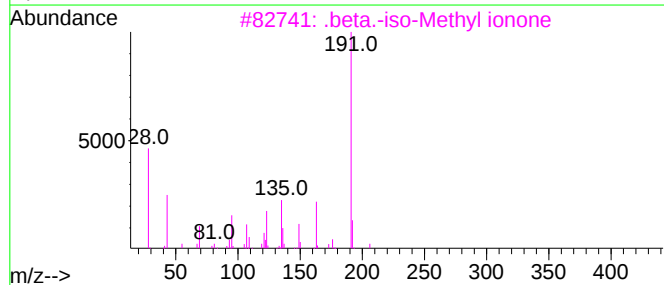
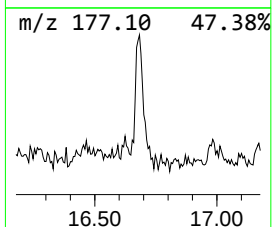
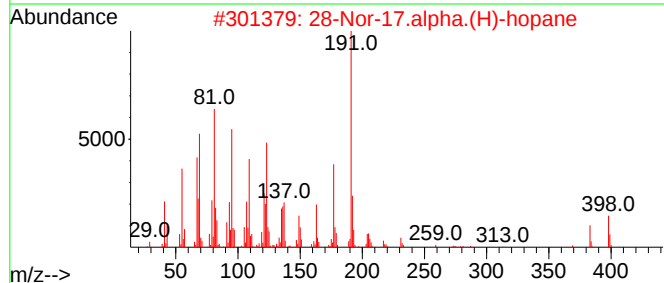
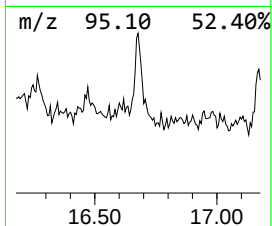
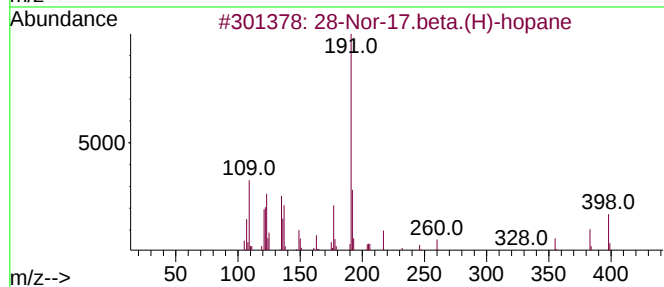
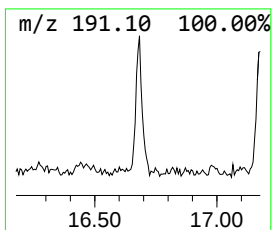
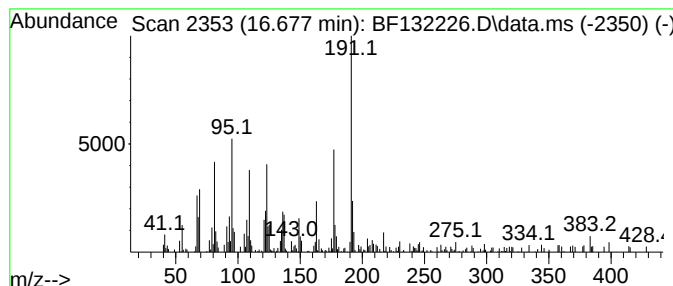
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 28-Nor-17.beta.(H)-hopane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	3.36 ng	186665	Perylene-d12	15.877

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	62
2			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	60
3			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
4			Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	49
5			Silane, dimethyldi(2-isopropylph...	328	C20H28O2Si	1000347-25-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
Data File : BF132226.D
Acq On : 30 Jan 2023 23:31
Operator : CG\JU
Sample : 01328-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-BORING-1-0-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012723.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-...	5.331	36.1	ng	2107700	1	7.078	1166510	20.0
Benzophenone	10.842	2.8	ng	237361	3	10.131	1676690	20.0
n-Hexadecanoic ...	12.136	4.4	ng	314810	4	11.624	1439200	20.0
4,4'-Bis(tetra...	13.077	2.2	ng	120249	5	14.289	1111370	20.0
Tricosane	14.430	2.6	ng	142616	5	14.289	1111370	20.0
1,3-Benzenedica...	14.924	38.2	ng	2124000	5	14.289	1111370	20.0
Eicosane	15.465	2.6	ng	145813	6	15.877	1112260	20.0
28-Nor-17.beta....	16.677	3.4	ng	186665	6	15.877	1112260	20.0