

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
 Data File : BF131007.D
 Acq On : 05 Nov 2022 00:10
 Operator : CG\JU
 Sample : N5318-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20221106-COMP-05

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131007.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	15	23	31	rVB	542465	703323	31.77%	3.974%
2	2.334	38	42	48	rVB	43352	55135	2.49%	0.311%
3	5.140	514	519	531	rVB	441537	523056	23.62%	2.955%
4	5.534	581	586	589	rBV	2184267	1962204	88.62%	11.086%
5	6.534	751	756	759	rBV	1941369	2052037	92.68%	11.593%
6	6.910	816	820	823	rBV	651658	505188	22.82%	2.854%
7	7.475	911	916	919	rBV	1392091	1307866	59.07%	7.389%
8	7.980	998	1002	1005	rBV	28972	24083	1.09%	0.136%
9	8.092	1018	1021	1034	rBV	97106	177585	8.02%	1.003%
10	8.192	1034	1038	1042	rVB	687197	658959	29.76%	3.723%
11	9.275	1216	1222	1225	rBV	2459252	2204645	99.58%	12.456%
12	9.345	1231	1234	1237	rVB2	30442	25100	1.13%	0.142%
13	9.957	1333	1338	1341	rVB	937593	757381	34.21%	4.279%
14	10.745	1468	1472	1476	rBV	1604895	1448654	65.43%	8.184%
15	10.869	1489	1493	1500	rVB4	22878	43869	1.98%	0.248%
16	11.321	1567	1570	1574	rVB3	28882	32208	1.45%	0.182%
17	11.451	1588	1592	1595	rBV	931254	818470	36.97%	4.624%
18	11.516	1599	1603	1606	rVB3	43181	41519	1.88%	0.235%
19	12.898	1835	1838	1841	rBV2	25010	27313	1.23%	0.154%
20	12.927	1841	1843	1848	rVB	53819	43751	1.98%	0.247%
21	13.039	1858	1862	1865	rBV	2505927	2214054	100.00%	12.509%
22	13.263	1897	1900	1903	rBV	42062	34000	1.54%	0.192%
23	13.504	1937	1941	1949	rVB3	34554	50153	2.27%	0.283%
24	13.604	1954	1958	1961	rBV2	61283	63865	2.88%	0.361%
25	13.933	2011	2014	2019	rVB	72079	60112	2.72%	0.340%
26	13.998	2019	2025	2036	rBV4	43191	134644	6.08%	0.761%
27	14.098	2038	2042	2047	rVB	764181	648651	29.30%	3.665%
28	14.192	2053	2058	2065	rBV	104679	109821	4.96%	0.620%
29	14.251	2065	2068	2071	rBV	62188	53909	2.43%	0.305%
30	14.557	2117	2120	2124	rVB	57248	52536	2.37%	0.297%
31	14.874	2170	2174	2178	rBV	42393	46395	2.10%	0.262%
32	14.957	2185	2188	2192	rVB2	47703	47715	2.16%	0.270%
33	15.227	2230	2234	2239	rVB2	40037	45827	2.07%	0.259%
34	15.604	2292	2298	2311	rVB	407280	567284	25.62%	3.205%
35	16.074	2374	2378	2386	rVB2	30603	53774	2.43%	0.304%
36	16.615	2464	2470	2483	rBV7	35498	104923	4.74%	0.593%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

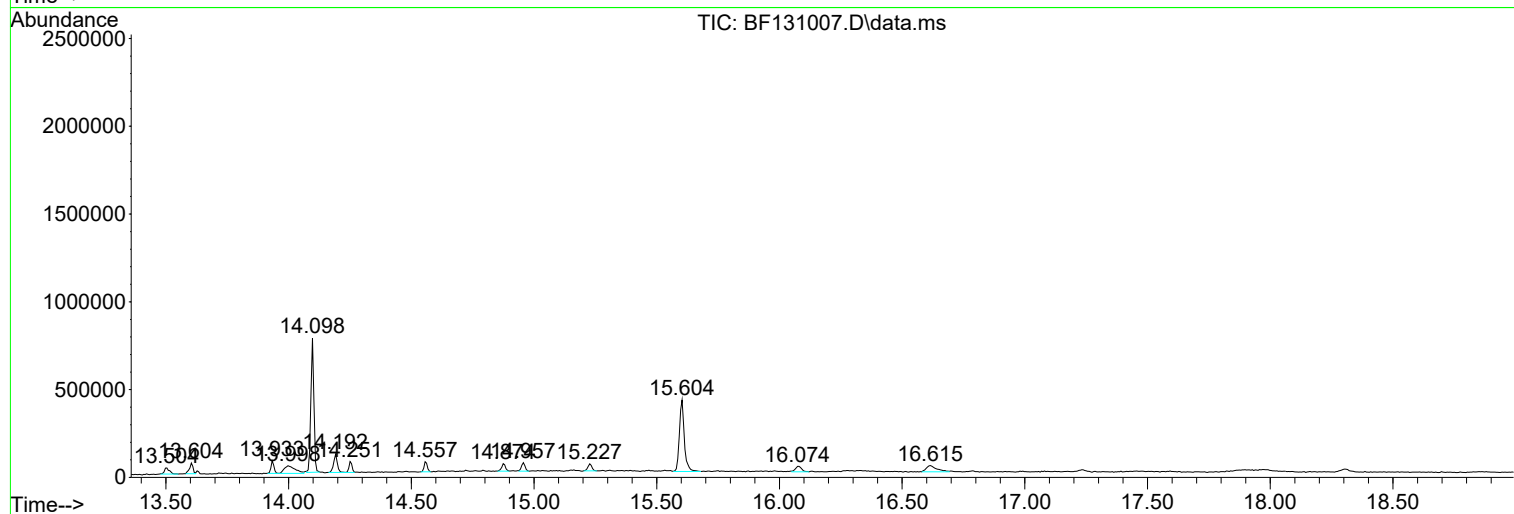
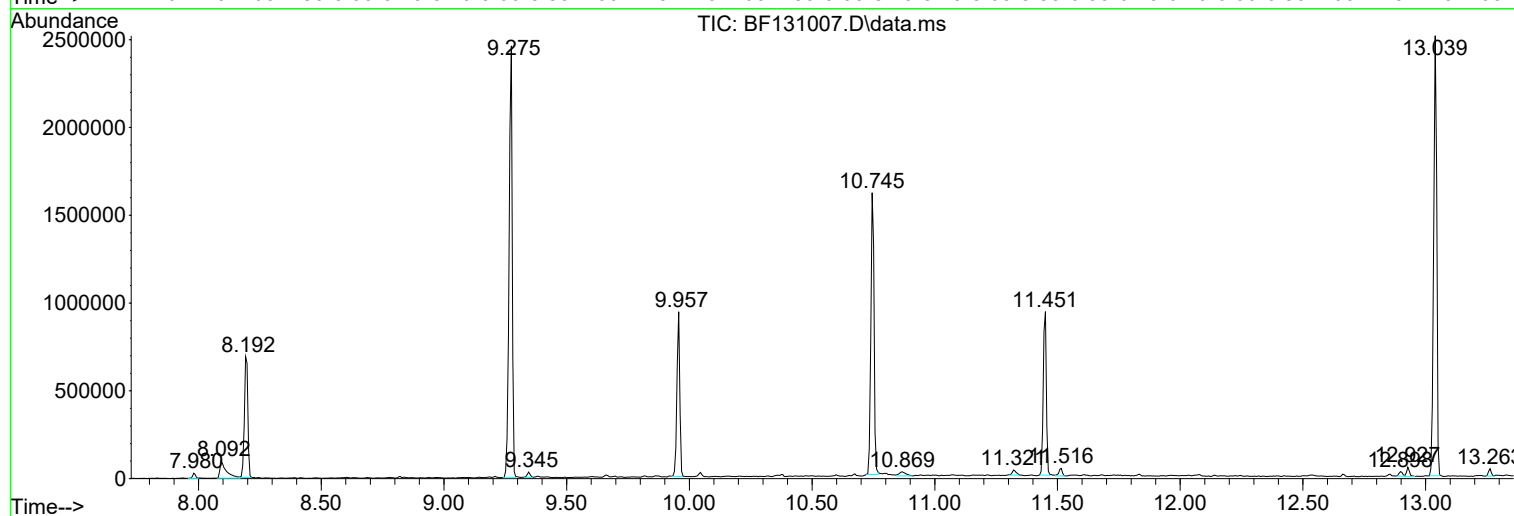
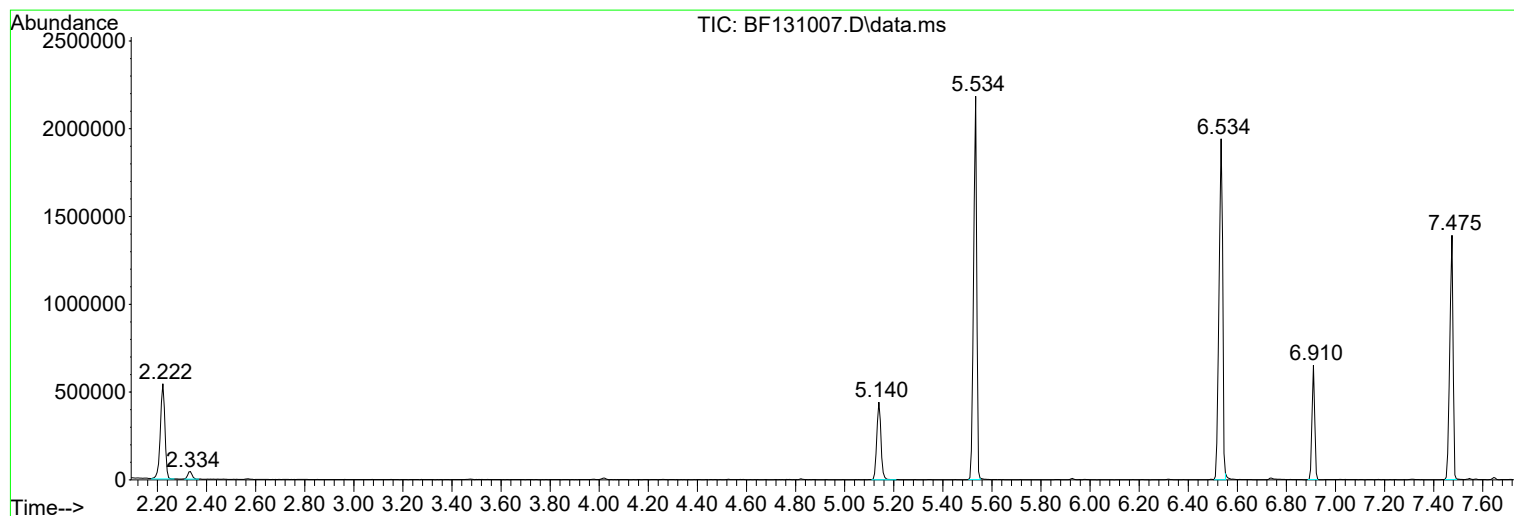
Sum of corrected areas: 17700009

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

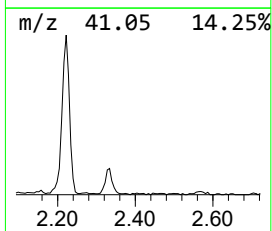
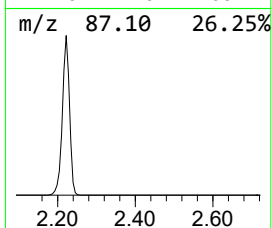
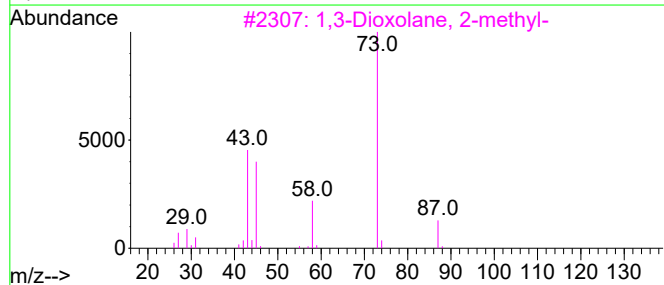
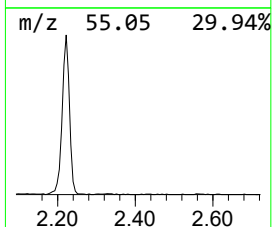
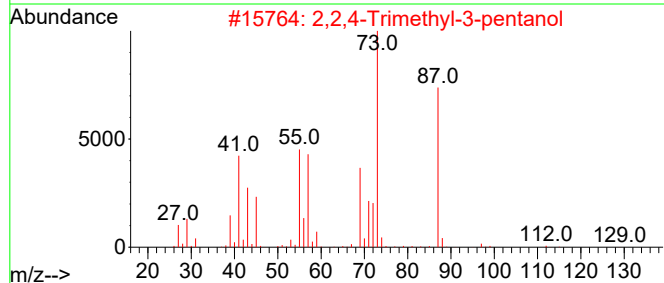
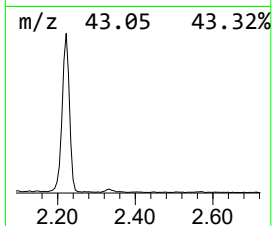
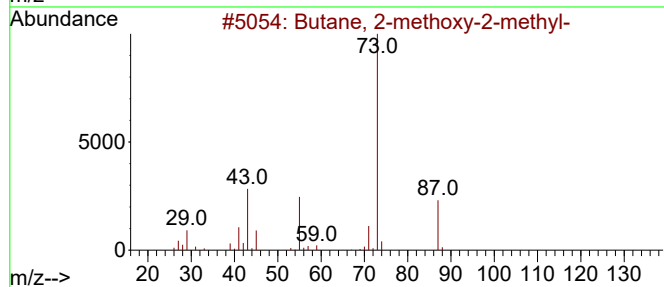
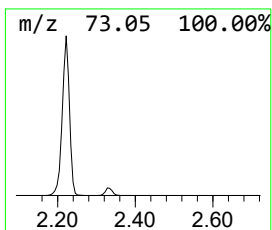
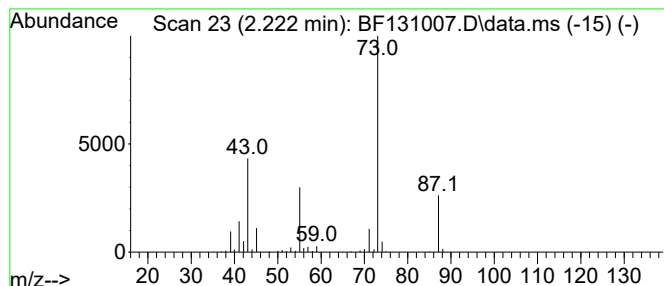
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	27.84 ng	703323	1,4-Dichlorobenzene-d4	6.910

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

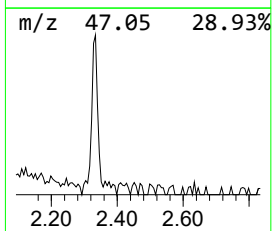
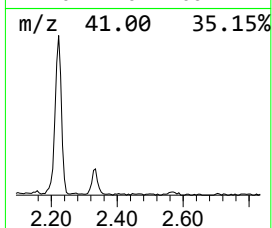
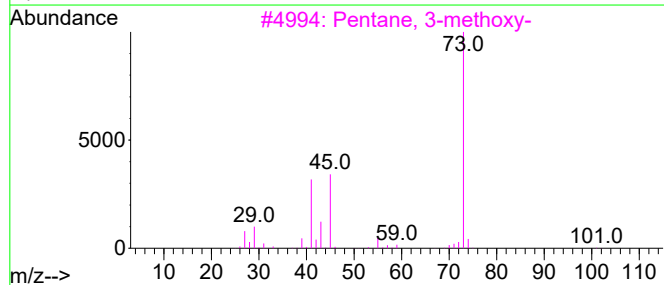
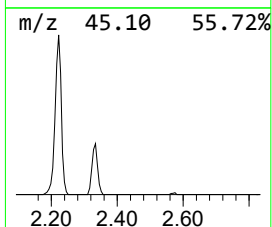
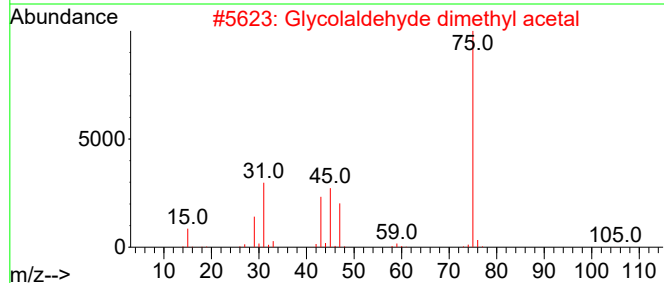
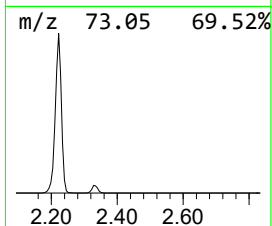
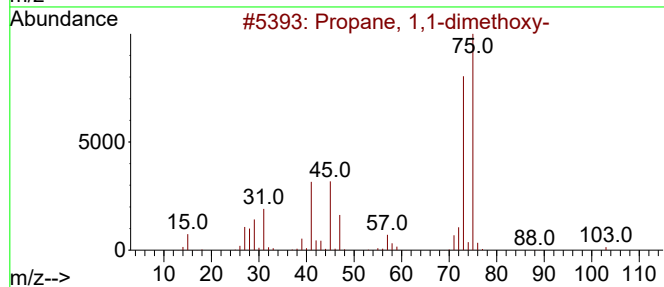
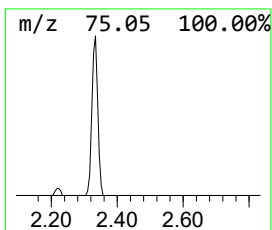
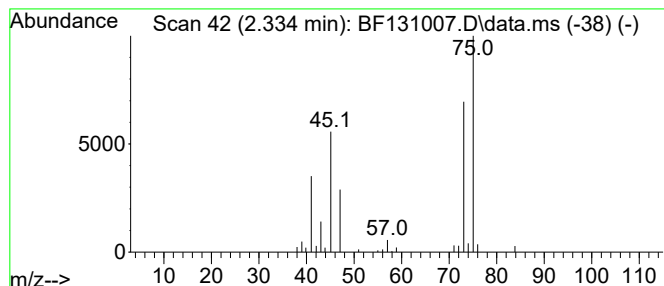
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	2.18 ng	55135	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5			5-Hexen-2-ol	100	C6H12O	000626-94-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

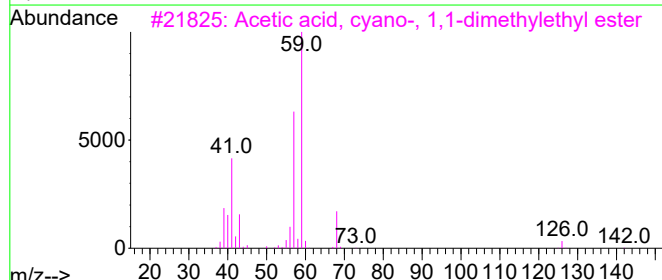
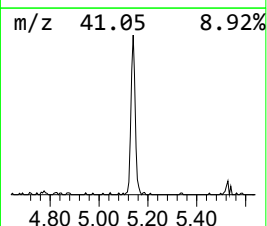
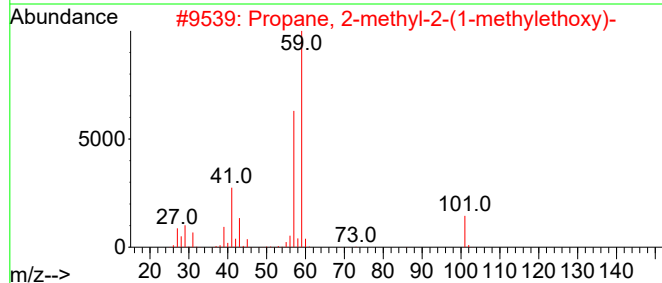
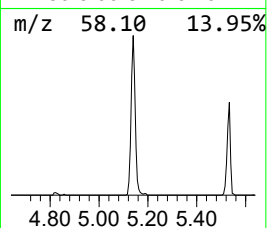
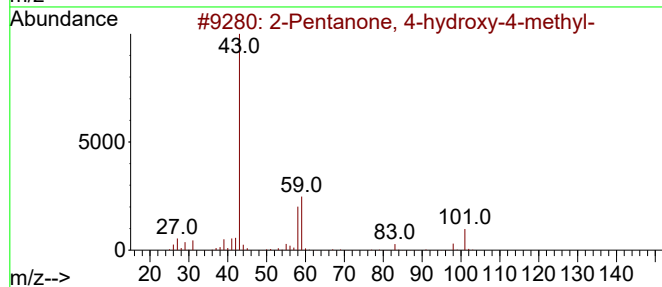
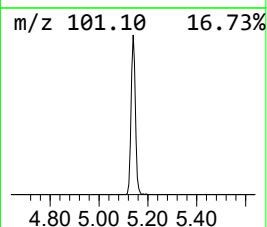
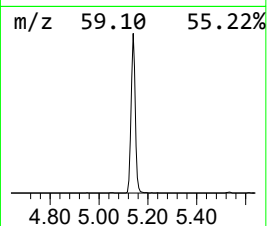
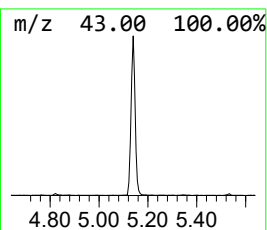
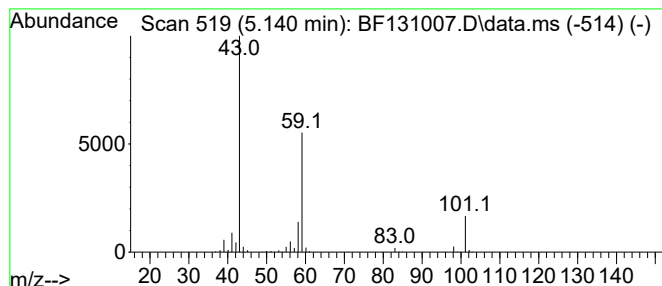
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	20.71 ng	523056	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

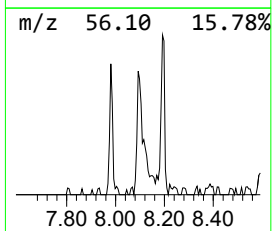
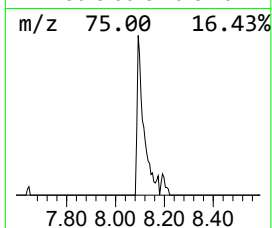
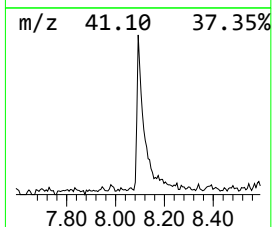
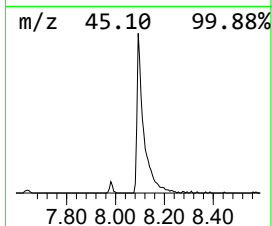
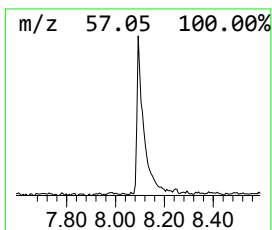
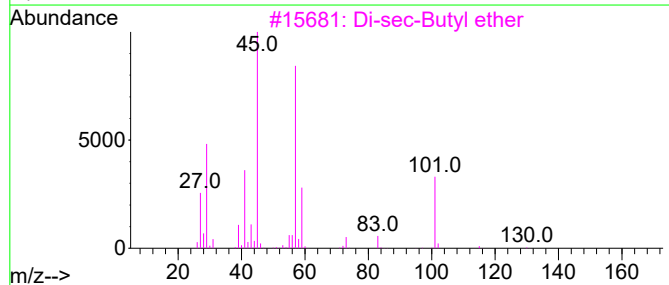
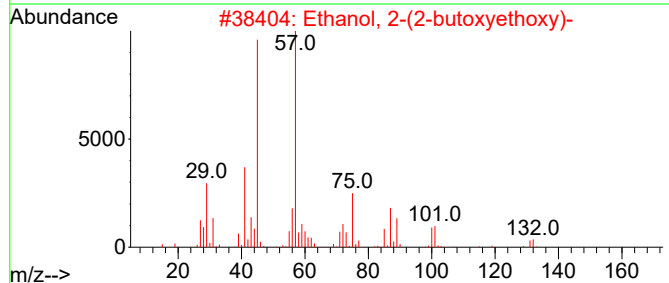
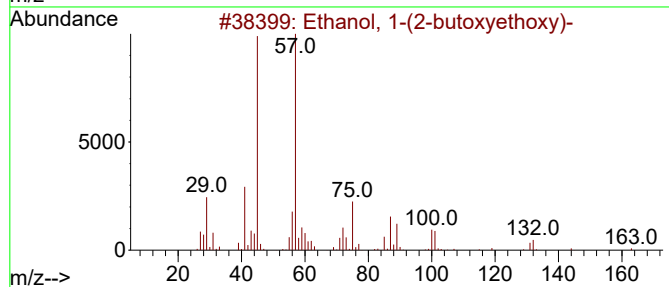
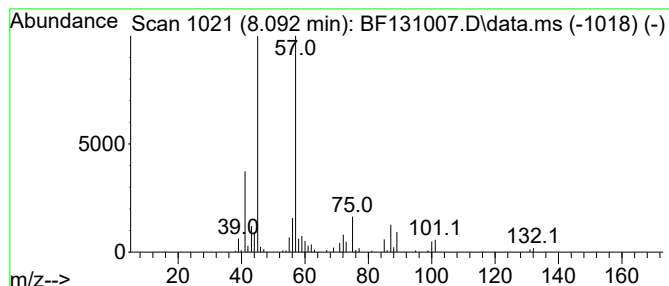
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	5.39 ng	177585	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

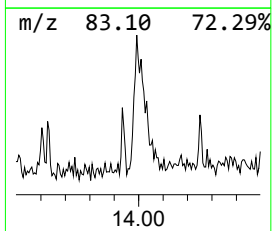
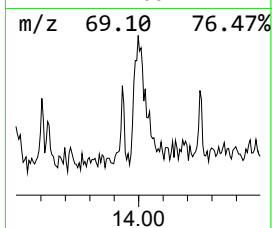
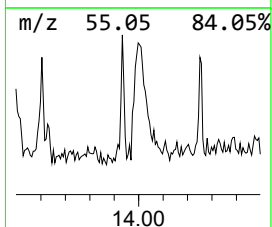
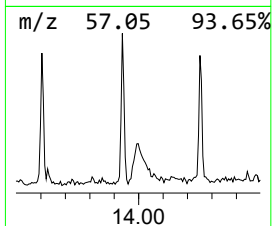
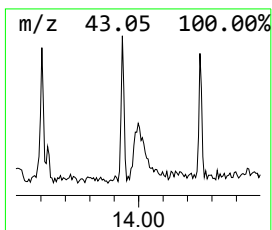
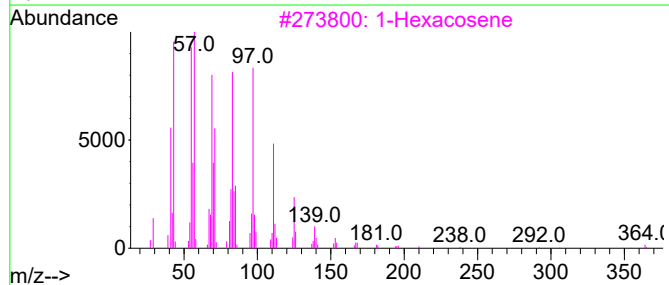
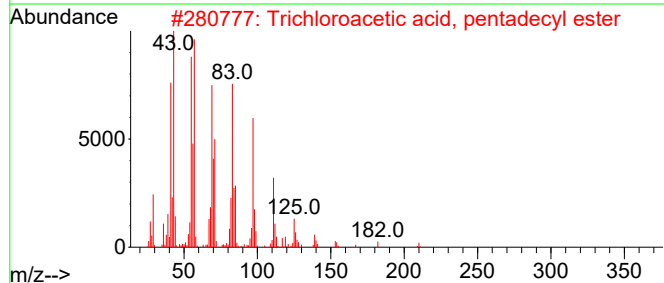
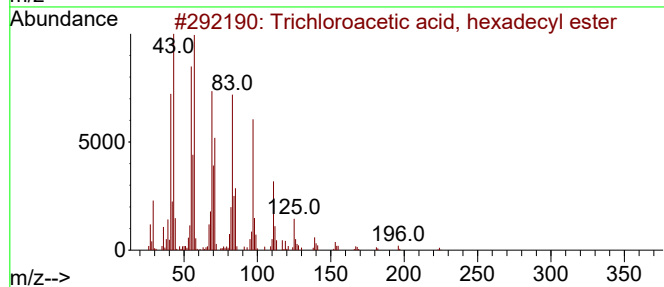
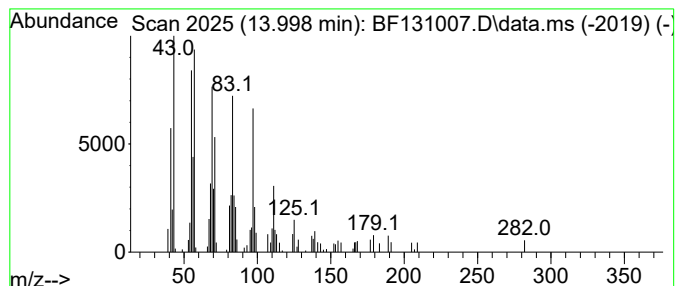
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	4.15 ng	134644	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

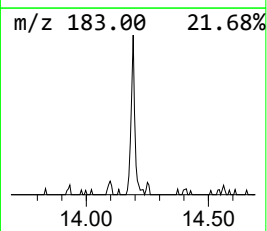
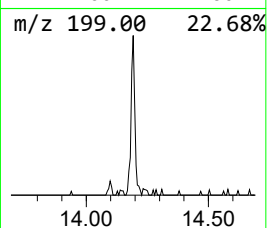
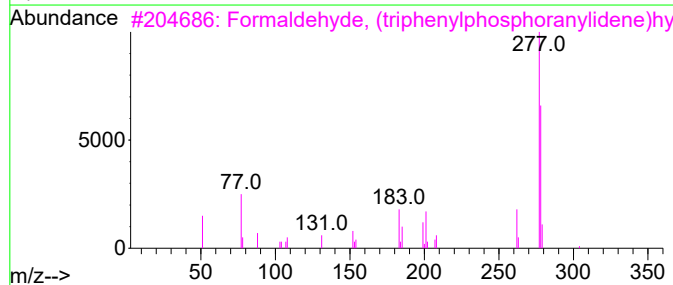
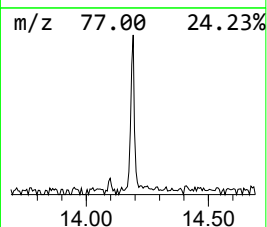
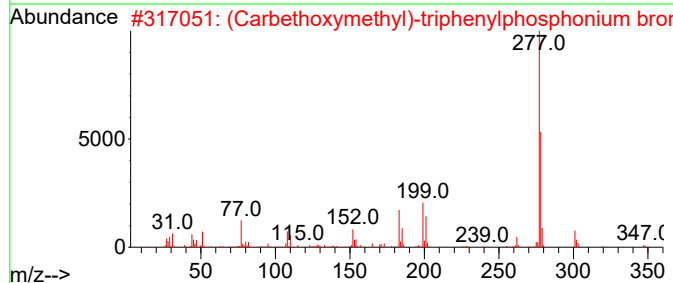
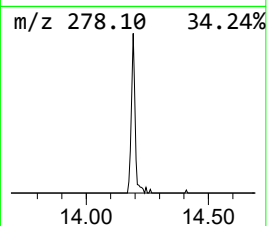
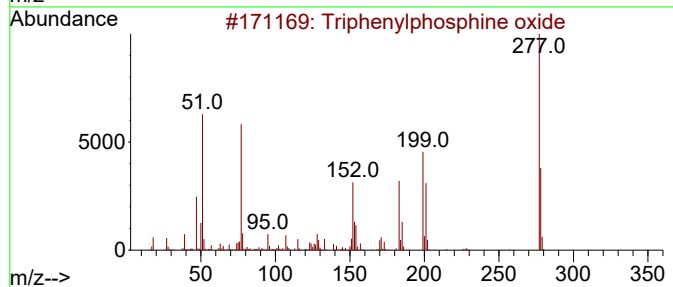
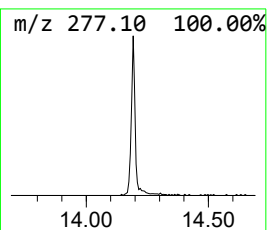
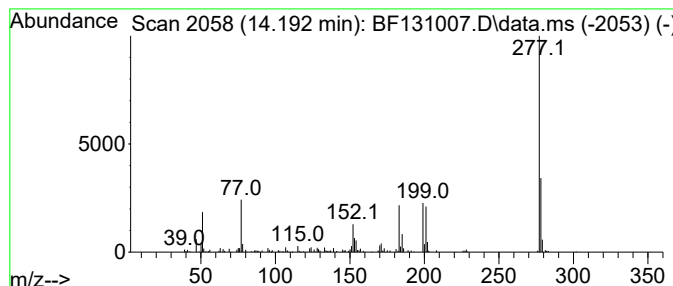
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.39 ng	109821	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	53
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

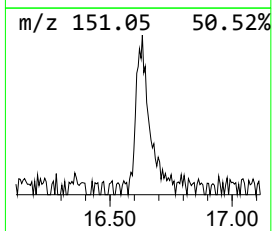
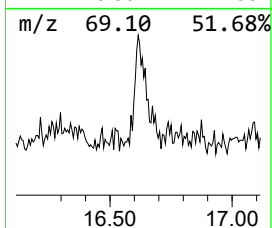
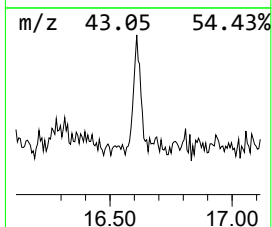
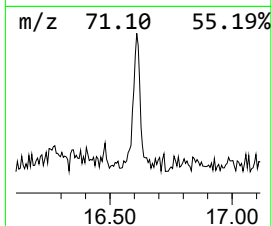
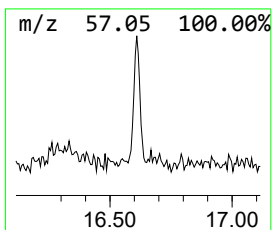
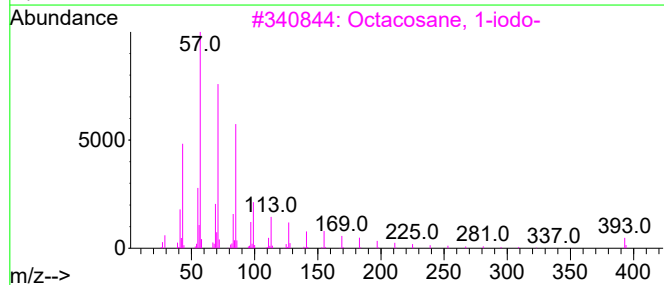
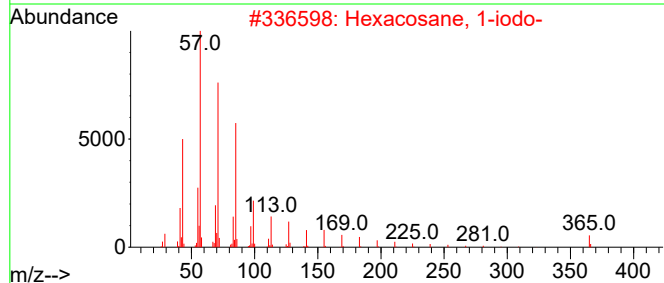
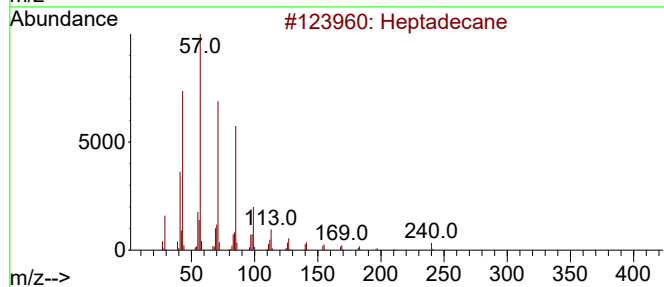
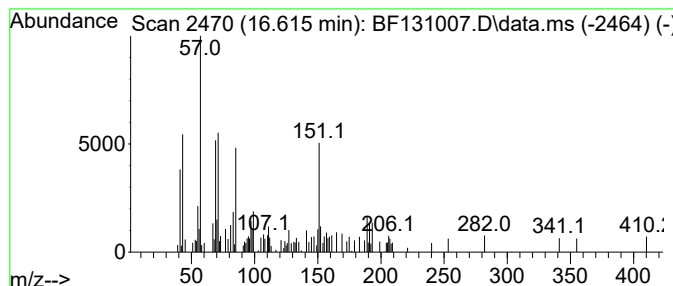
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.615	3.70 ng	104923	Perylene-d12	15.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	55
2		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	43
3		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	43
4		Tricosane	324	C23H48	000638-67-5	43
5		Octacosane	394	C28H58	000630-02-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131007.D
Acq On : 05 Nov 2022 00:10
Operator : CG\JU
Sample : N5318-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221106-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.222	27.8	ng	703323	1	6.910	505188	20.0
Propane, 1,1-di...	2.334	2.2	ng	55135	1	6.910	505188	20.0
2-Pentanone, 4-...	5.140	20.7	ng	523056	1	6.910	505188	20.0
Ethanol, 1-(2-b...	8.092	5.4	ng	177585	2	8.192	658959	20.0
Trichloroacetic...	13.998	4.2	ng	134644	5	14.098	648651	20.0
Triphenylphosph...	14.192	3.4	ng	109821	5	14.098	648651	20.0
Heptadecane	16.615	3.7	ng	104923	6	15.604	567284	20.0