LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUM-13

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: BF127218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.504	542	547	550	rBV	2299151	2074018	79.85%	11.211%
2	6.510	713	718	731	rVB	2059921	2231732	85.92%	12.063%
3	6.875	777	780	784	rVB	595819	493249	18.99%	2.666%
4	7.445	871	877	880	rBV	1566085	1461062	56.25%	7.897%
5	8.081	978	985	995	rBV6	23715	83870	3.23%	0.453%
6	8.163	995	999	1002	rVV	757220	665058	25.60%	3.595%
7	9.239	1176	1182	1185	rBV	3111074	2597503	100.00%	14.040%
8	9.922	1294	1298	1301	rVB	804967	704405	27.12%	3.808%
9	10.716	1428	1433	1436	rBV	2005978	1839737	70.83%	9.944%
10	11.351	1537	1541	1545	rBV	61567	57857	2.23%	0.313%
11	11.410	1547	1551	1554	rVV	927793	788068	30.34%	4.260%
12	11.433	1554	1555	1558	rVV	148023	94290	3.63%	0.510%
13	11.486	1560	1564	1567	rVB	29378	31590	1.22%	0.171%
14	11.569	1574	1578	1584	rBV	44289	50609	1.95%	0.274%
15	11.927	1631	1639	1643	rBV5	35668	79758	3.07%	0.431%
16	11.963	1643	1645	1648	rVB	46557	35100	1.35%	0.190%
17	12.139	1673	1675	1679	rBV4	36668	31268	1.20%	0.169%
18	12.180	1679	1682	1684	rVB	43880	37956	1.46%	0.205%
19	12.627	1754	1758	1761	rBV	245677	204842	7.89%	1.107%
20	12.716	1770	1773	1776	rVB	67211	53223	2.05%	0.288%
21	12.816	1786	1790	1792	rBV3	68992	74932	2.88%	0.405%
22	12.857	1795	1797	1800	rVB	179531	138946	5.35%	0.751%
23	12.998	1817	1821	1824	rBV	2611111	2281889	87.85%	12.334%
24	13.186	1850	1853	1856	rVB	36651	34955	1.35%	0.189%
25	13.510	1905	1908	1913	rVB5	20929	29923	1.15%	0.162%
26	13.839	1960	1964	1968	rBV3	31566	55044	2.12%	0.298%
27	13.880	1968	1971	1974	rVV3	48635	76942	2.96%	0.416%
28	13.921	1974	1978	1984	rVV	166227	204270	7.86%	1.104%
29	14.010	1984	1993	1994	rVV6	34367	86045	3.31%	0.465%
30	14.057	1997	2001	2004	rVV2	539463	564355	21.73%	3.051%
31	14.080	2004	2005	2013	rVV	100652	81057	3.12%	0.438%
32	14.151	2013	2017	2022	rVB2	81283	93956	3.62%	0.508%
33	14.510	2075	2078	2085	rBV4	23036	45366	1.75%	0.245%
34	14.592	2085	2092	2096	rVV6	26357	47776	1.84%	0.258%
35	15.104	2175	2179	2183	rBV	87216	135996	5.24%	0.735%
36	15.257	2201	2205	2209	rBV4	19185	30856	1.19%	0.167%

LSC Area Percent Report

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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

37	15.315	2211	2215	2223	rBV8	25713	50866	1.96%	0.275%
38	15.415	2229	2232	2239	rVB	44712	57193	2.20%	0.309%
39	15.480	2239	2243	2249	rVB	70648	93489	3.60%	0.505%
40	15.551	2249	2255	2259	rBV	349242	465198	17.91%	2.515%
41	15.998	2327	2331	2336	rBV3	26364	50052	1.93%	0.271%
42	17.051	2506	2510	2519	rVB4	37268	79393	3.06%	0.429%
43	18.221	2704	2709	2715	rVB8	24965	52865	2.04%	0.286%
44	18.962	2827	2835	2836	rBV7	29011	53837	2.07%	0.291%

Sum of corrected areas: 18500396

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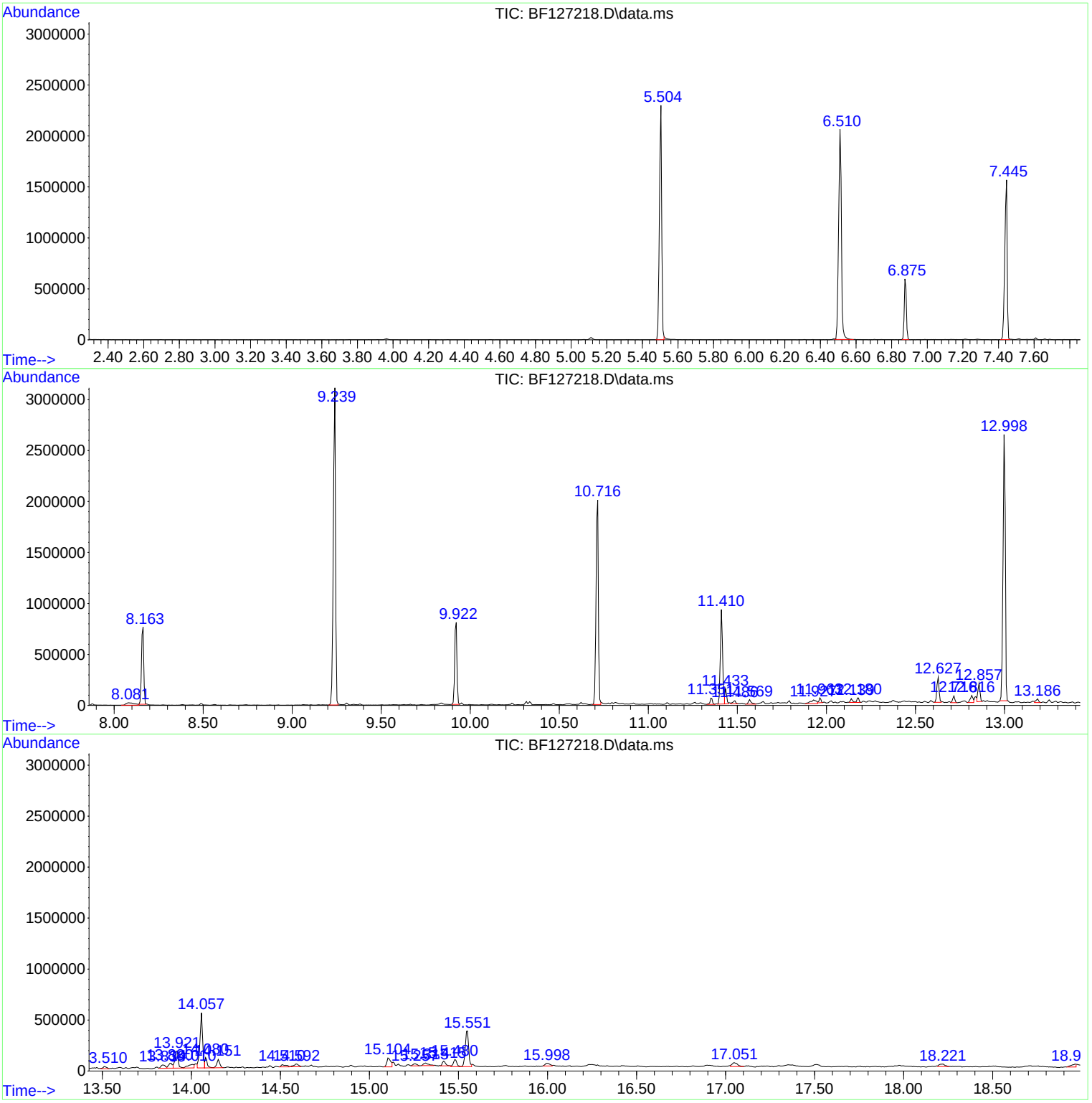
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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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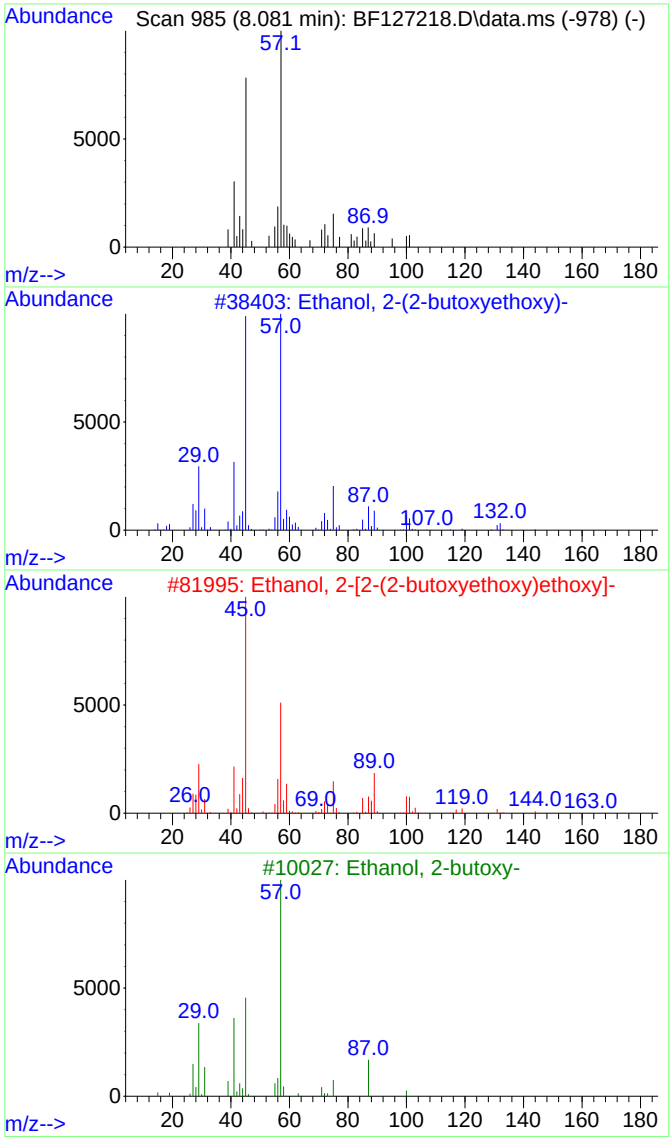
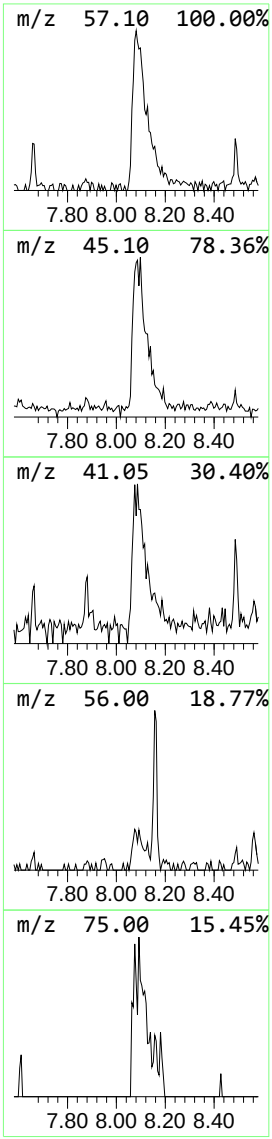
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	2.52 ng	83870	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45
5	2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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

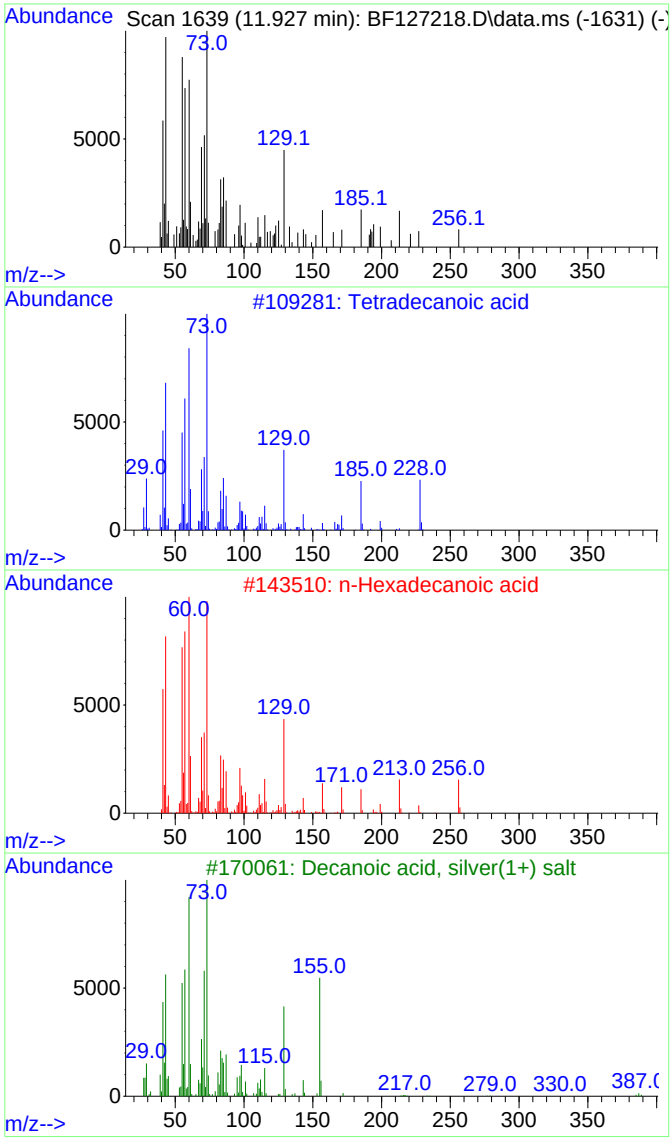
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

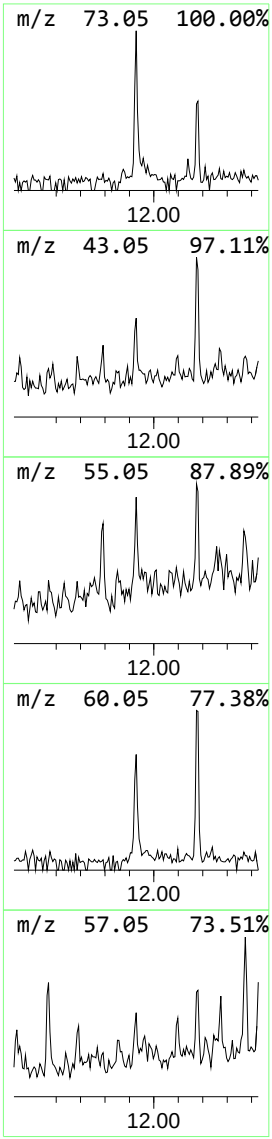
****

Peak Number 2 Tetradecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.02 ng	79758	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

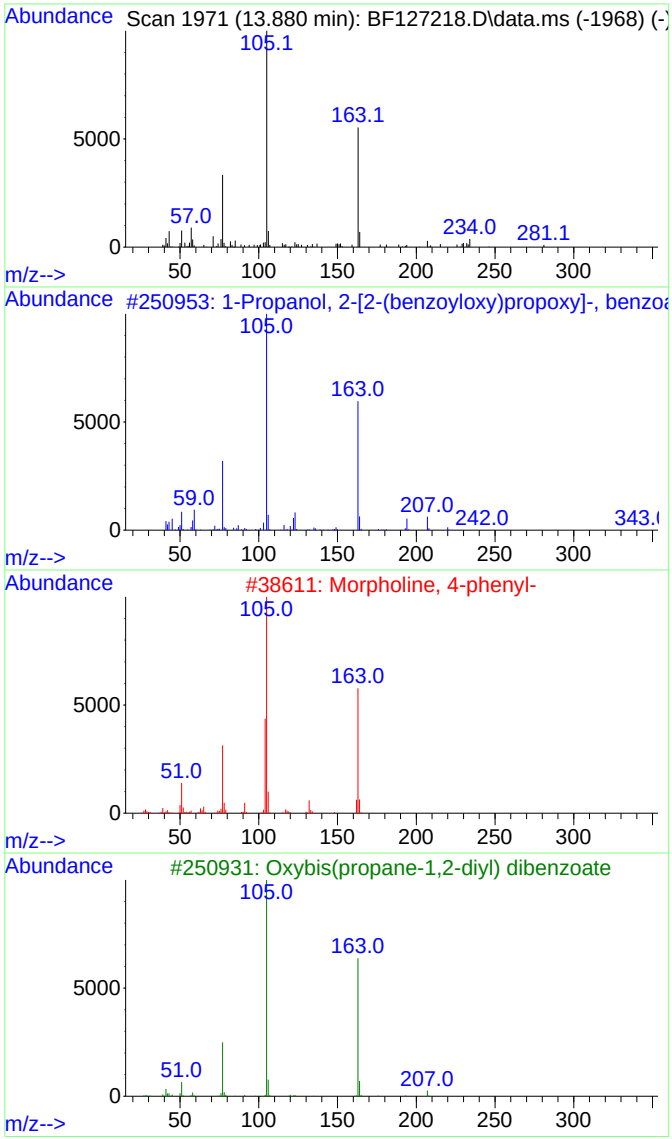
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

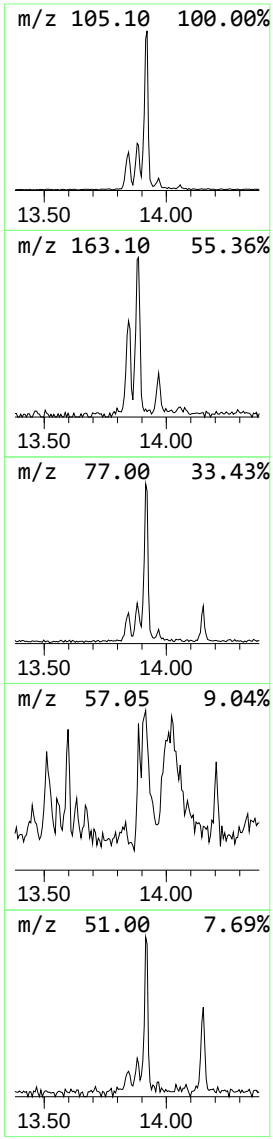
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol, 2-[2-(benzoylox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.73 ng	76942	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	64
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	53
4	6H-1,3,4-Oxadiazin-6-one, 5-tert...	230	C13H14N2O2	1000142-96-3	30
5	Phenylglyoxylic acid, 2-methylpr...	206	C12H14O3	1000453-47-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
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Operator : CG\JU
Sample : N1751-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
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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
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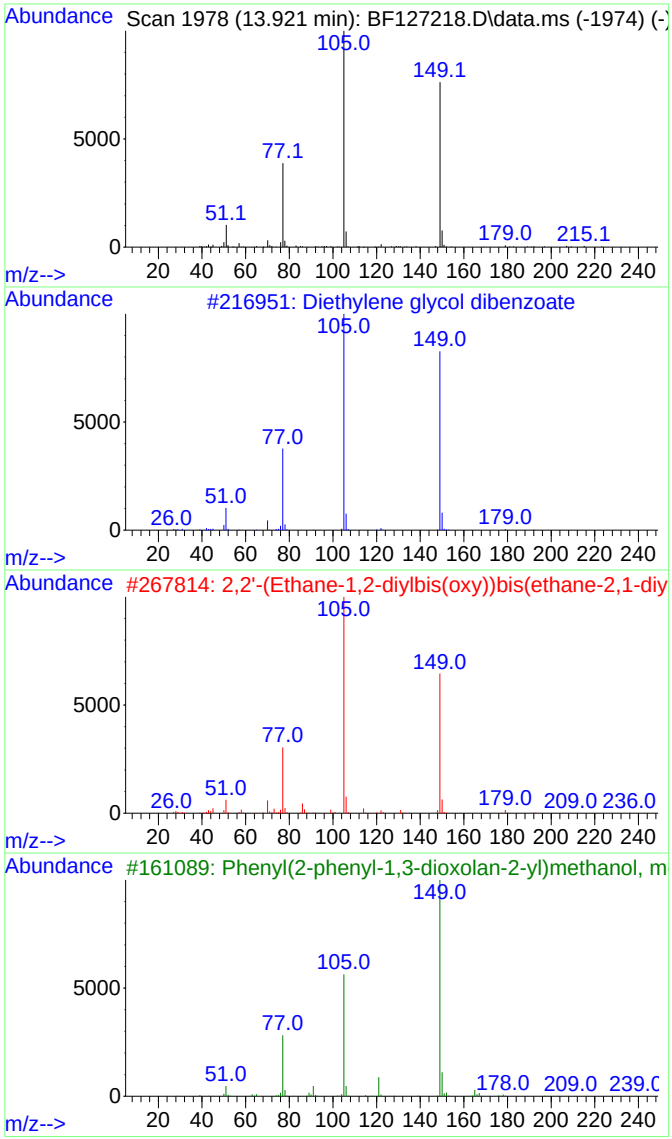
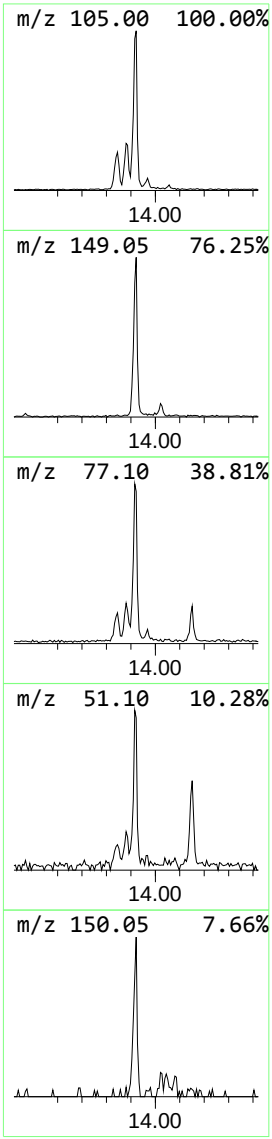
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	7.24 ng	204270	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52





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Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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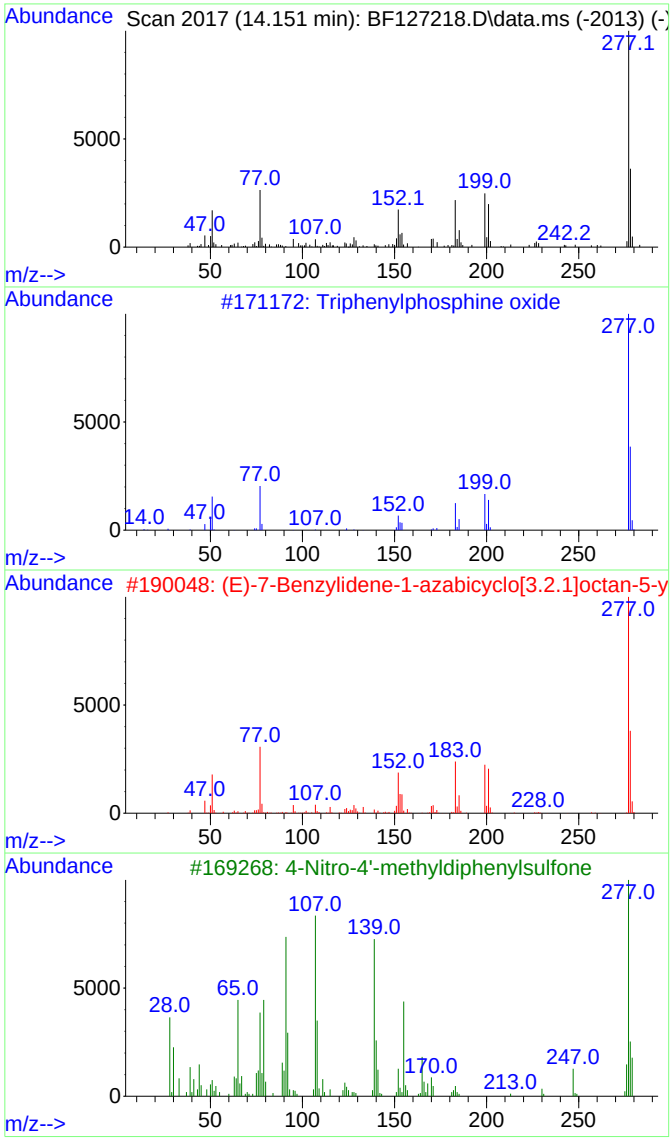
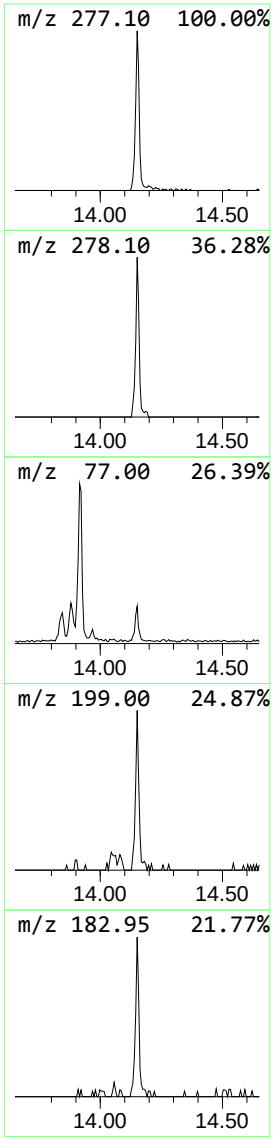
Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	3.33 ng	93956	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	91
3	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
5	Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	28





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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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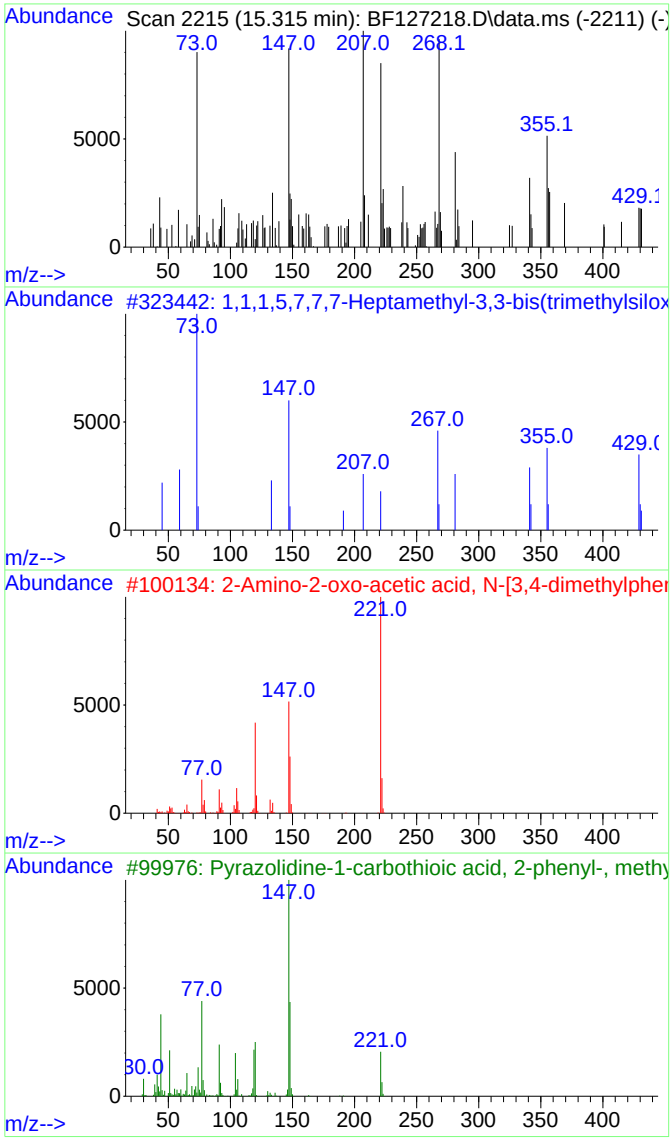
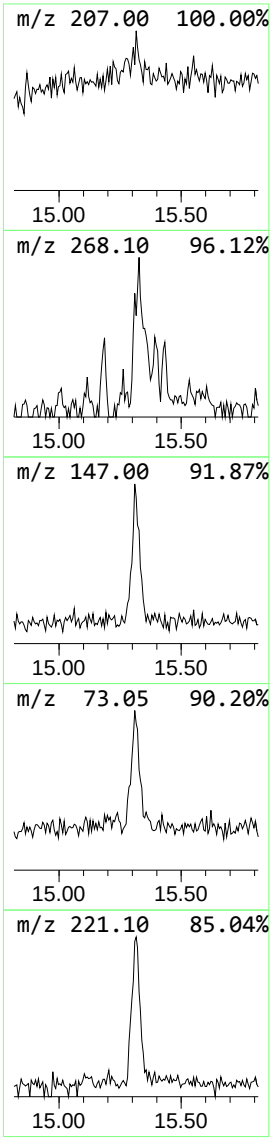
Peak Number 6 unknown15.315 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	2.19 ng	50866	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	25
2	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	22
3	Pyrazolidine-1-carbothioic acid,...	221	C11H15N3S	1000305-21-7	22
4	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	16
5	4-(4-Methylphenyl)-1-benzothioph...	268	C16H12O2S	100046-86-4	15





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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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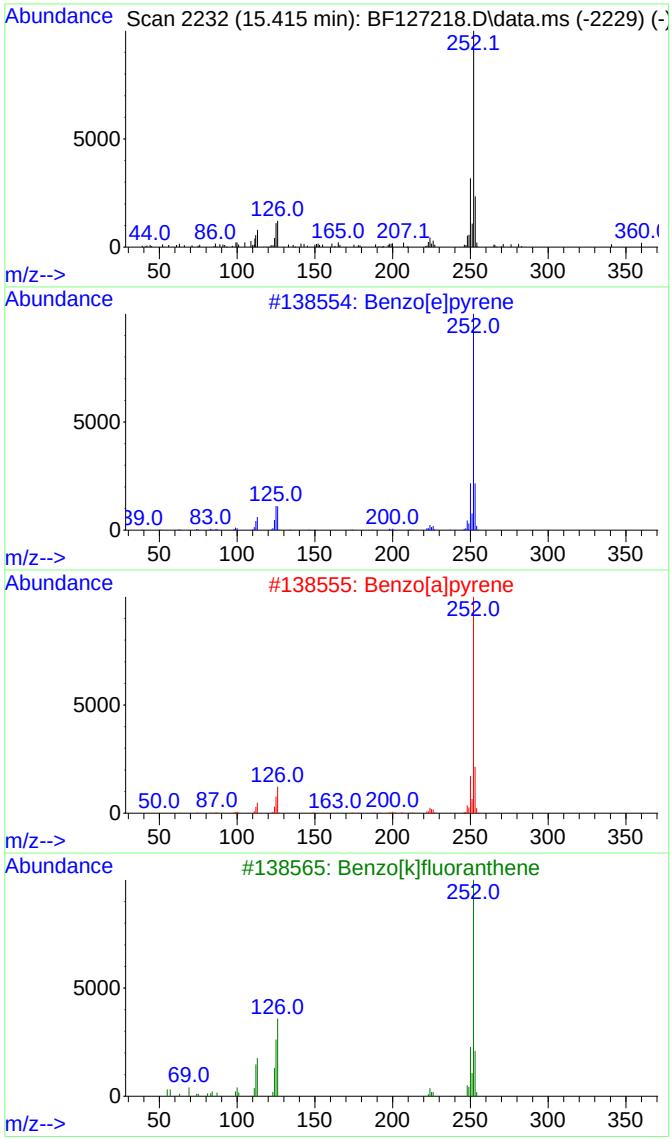
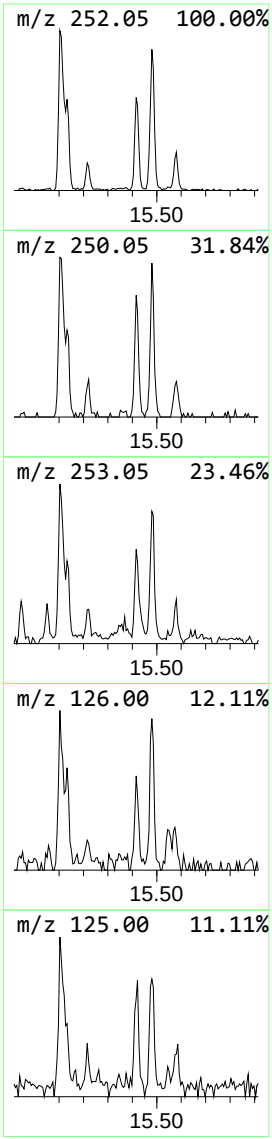
Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.415	2.46 ng	57193	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	90





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Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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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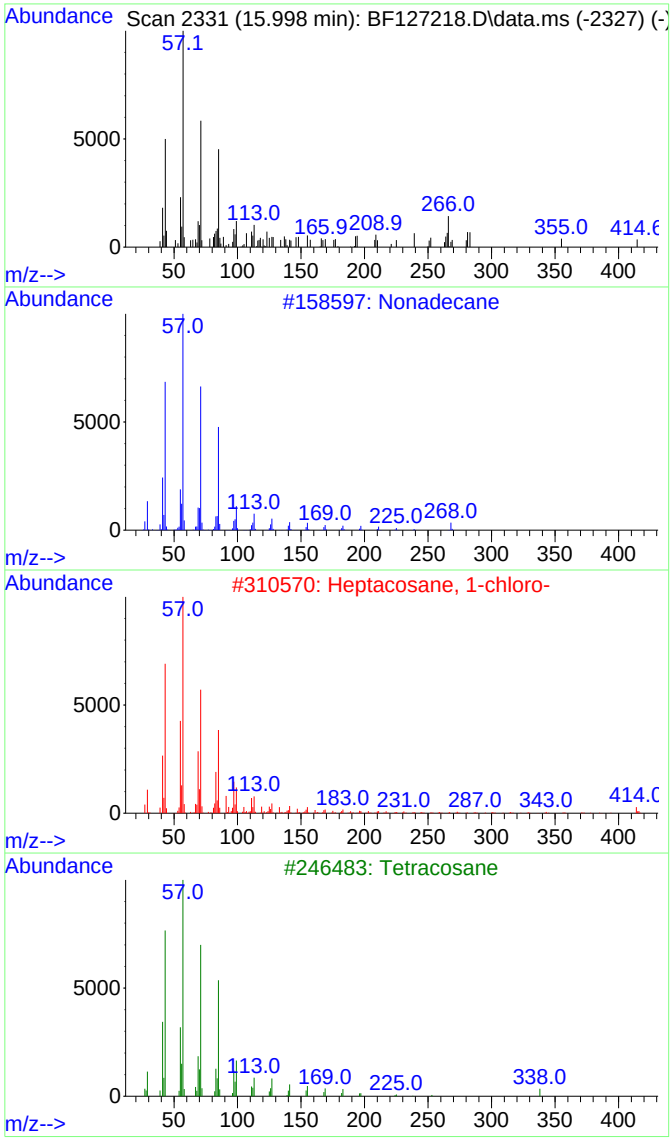
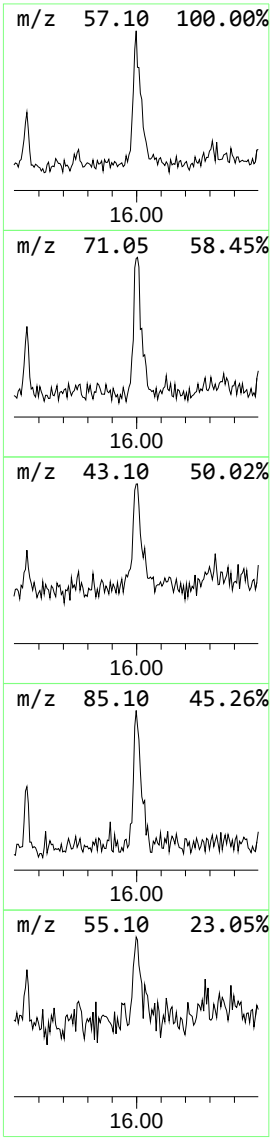
Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.15 ng	50052	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	92
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
3	Tetracosane	338	C24H50	000646-31-1	53
4	Heptadecane	240	C17H36	000629-78-7	53
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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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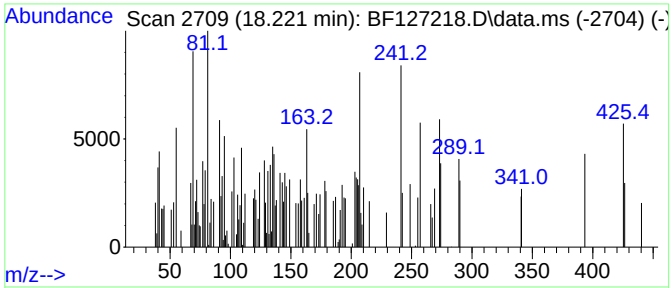
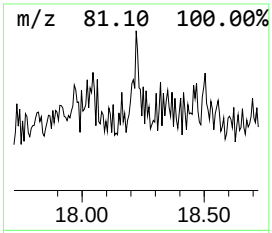
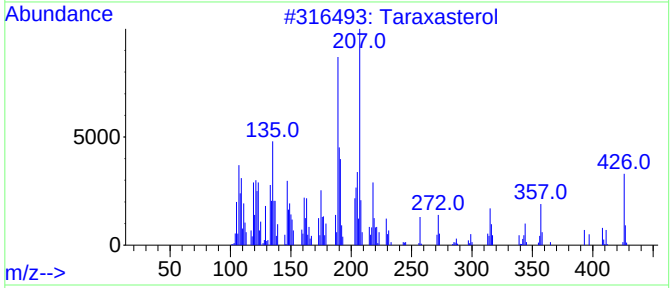
Peak Number 10 unknown18.221 Concentration Rank 8

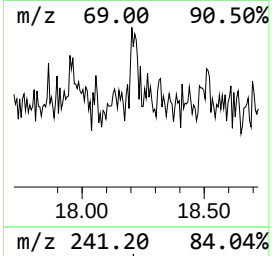
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	2.27 ng	52865	Perylene-d12	15.551

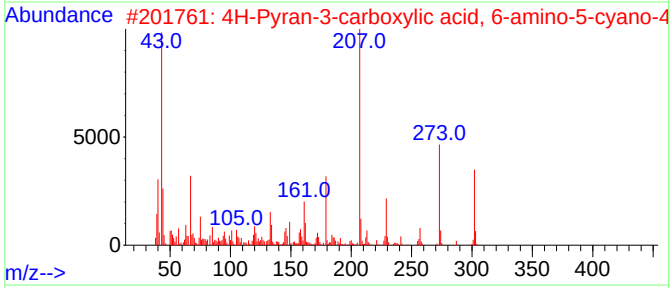
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Taraxasterol	426	C30H50O	001059-14-9	11
2	4H-Pyran-3-carboxylic acid, 6-am...	302	C16H15FN2O3	339060-50-3	10
3	Adamantane, 1-(4-methylphenylami...	241	C17H23N	019984-39-5	9
4	2-(Acridin-9-ylamino)-3-(3H-imid...	332	C19H16N4O2	1000285-93-8	9
5	Ethofumesate	286	C13H18O5S	026225-79-6	9

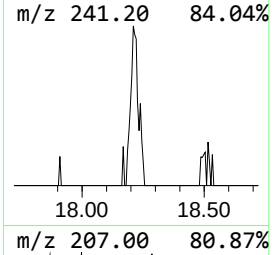


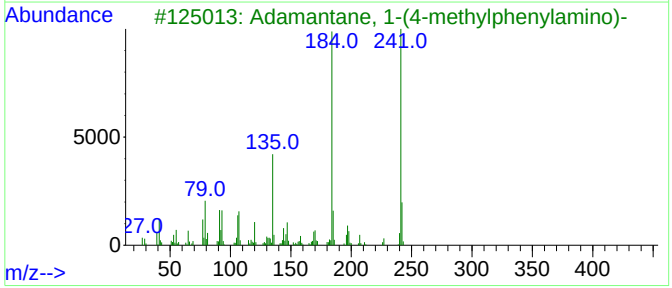


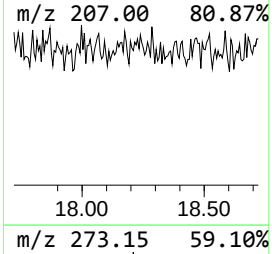


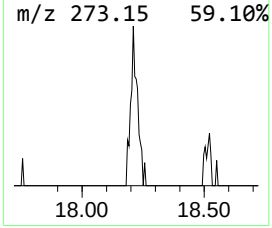












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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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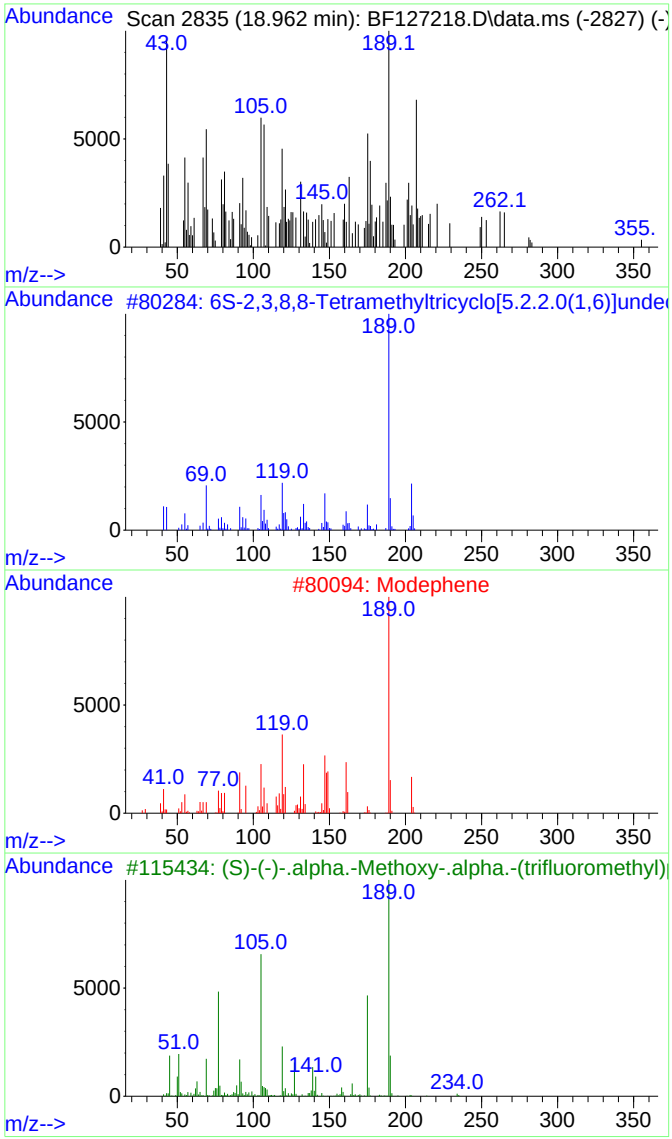
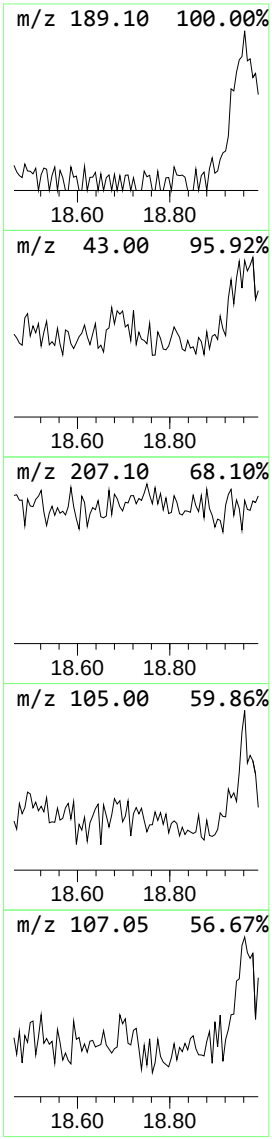
Peak Number 11 unknown18.962 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.962	2.31 ng	53837	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	38
2	Modephene	204	C15H24	068269-87-4	30
3	(S)-(-)-.alpha.-Methoxy-.alpha.-...	234	C10H9F3O3	017257-71-5	27
4	Benzeneacetic acid, .alpha.-meth...	234	C10H9F3O3	020445-31-2	27
5	1H-Pyrazol-3-amine, 4,5-dihydro-...	189	C11H15N3	1000327-38-2	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127218.D
Acq On : 07 Mar 2022 12:32
Operator : CG\JU
Sample : N1751-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-13

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.081	2.5	ng	83870	2	8.163	665058	20.0
Tetradecanoic acid	11.927	2.0	ng	79758	4	11.410	788068	20.0
1-Propanol, 2-[...	13.880	2.7	ng	76942	5	14.057	564355	20.0
Diethylene glyc...	13.921	7.2	ng	204270	5	14.057	564355	20.0
Triphenylphosph...	14.151	3.3	ng	93956	5	14.057	564355	20.0
unknown15.315	15.315	2.2	ng	50866	6	15.551	465198	20.0
Benzo[e]pyrene	15.415	2.5	ng	57193	6	15.551	465198	20.0
Nonadecane	15.998	2.1	ng	50052	6	15.551	465198	20.0
unknown18.221	18.221	2.3	ng	52865	6	15.551	465198	20.0
unknown18.962	18.962	2.3	ng	53837	6	15.551	465198	20.0