LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116753.D
Acq On : 1 Sep 2019 20:03
Operator : HP/JU
Sample : K4547-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	16	rBV	68603	92180	2.87%	0.439%
2	4.469	400	405	410	rBV	50676	77342	2.41%	0.368%
3	5.457	569	573	579	rBV	1705697	1563777	48.77%	7.446%
4	6.281	707	713	715	rBV2	86306	110268	3.44%	0.525%
5	6.475	741	746	751	rBV	1989336	1896067	59.13%	9.028%
6	6.616	765	770	773	rBV	2099876	1838416	57.34%	8.754%
7	6.845	805	809	812	rBV	676057	540723	16.86%	2.575%
8	6.904	815	819	826	rVB2	249779	307061	9.58%	1.462%
9	7.004	832	836	839	rBV	1690510	1409160	43.95%	6.710%
10	7.169	859	864	873	rBV4	42878	89129	2.78%	0.424%
11	7.245	873	877	880	rBV	165149	148607	4.63%	0.708%
12	7.404	896	904	907	rBV	1301154	1202101	37.49%	5.724%
13	8.128	1023	1027	1030	rBV	995318	767069	23.92%	3.652%
14	8.733	1124	1130	1134	rVB2	84235	104050	3.25%	0.495%
15	8.839	1145	1148	1152	rVB	143118	119023	3.71%	0.567%
16	8.880	1152	1155	1162	rBV	195899	214576	6.69%	1.022%
17	9.204	1204	1210	1213	rBV	2672692	2432728	75.87%	11.584%
18	9.592	1273	1276	1280	rVB	380225	314103	9.80%	1.496%
19	9.698	1291	1294	1297	rBV	363038	256293	7.99%	1.220%
20	9.880	1319	1325	1328	rBV	1190088	1020352	31.82%	4.858%
21	10.669	1455	1459	1462	rBV	1429884	1452459	45.30%	6.916%
22	11.369	1576	1578	1583	rVB	683208	618839	19.30%	2.947%
23	12.963	1847	1849	1856	rVB	1479402	1220747	38.07%	5.813%
24	13.998	2022	2025	2028	rBV	3234604	3206391	100.00%	15.267%

Sum of corrected areas: 21001461

LSC Report - Integrated Chromatogram

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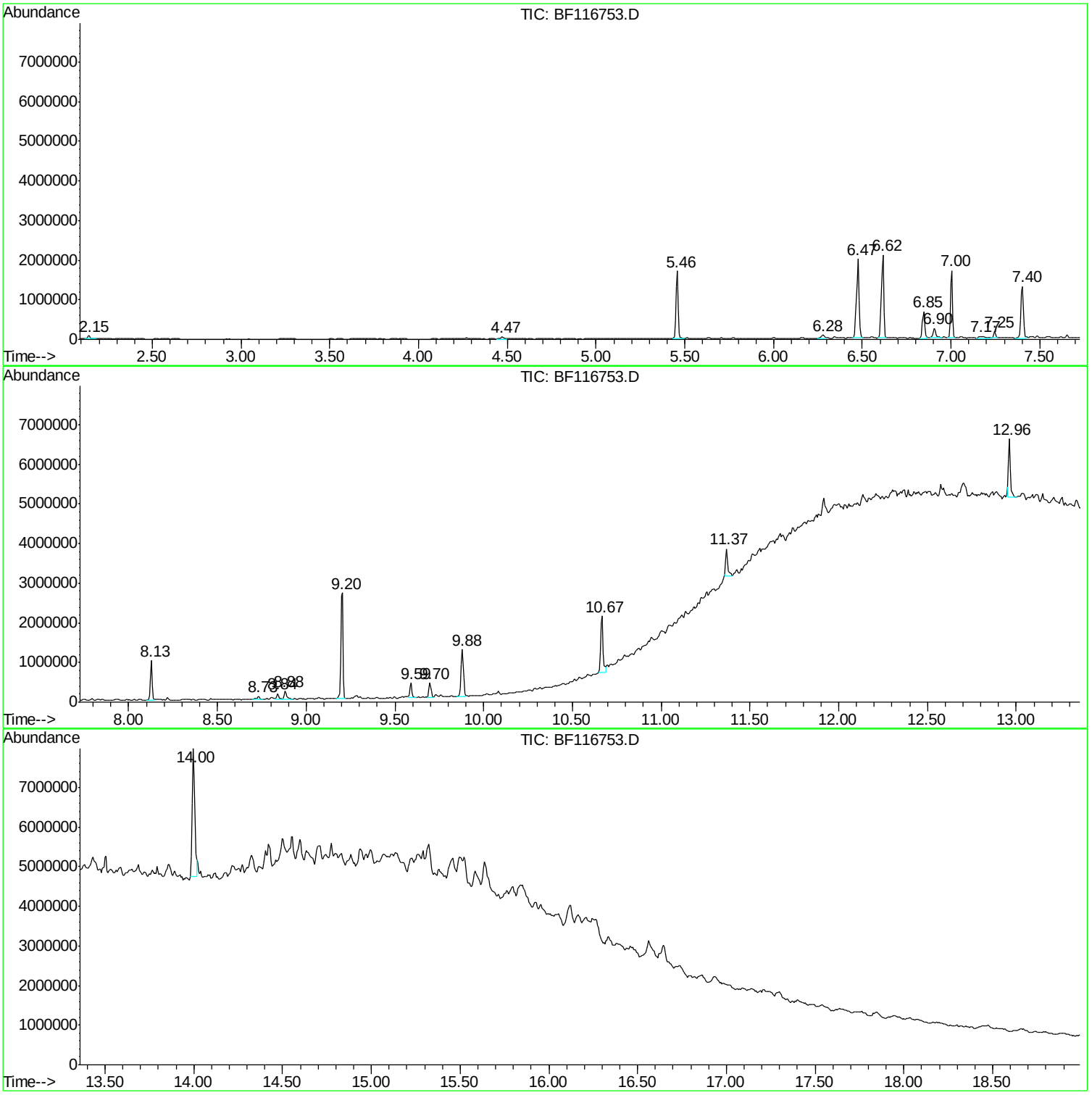
Sample : K4547-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Operator : HP/JU
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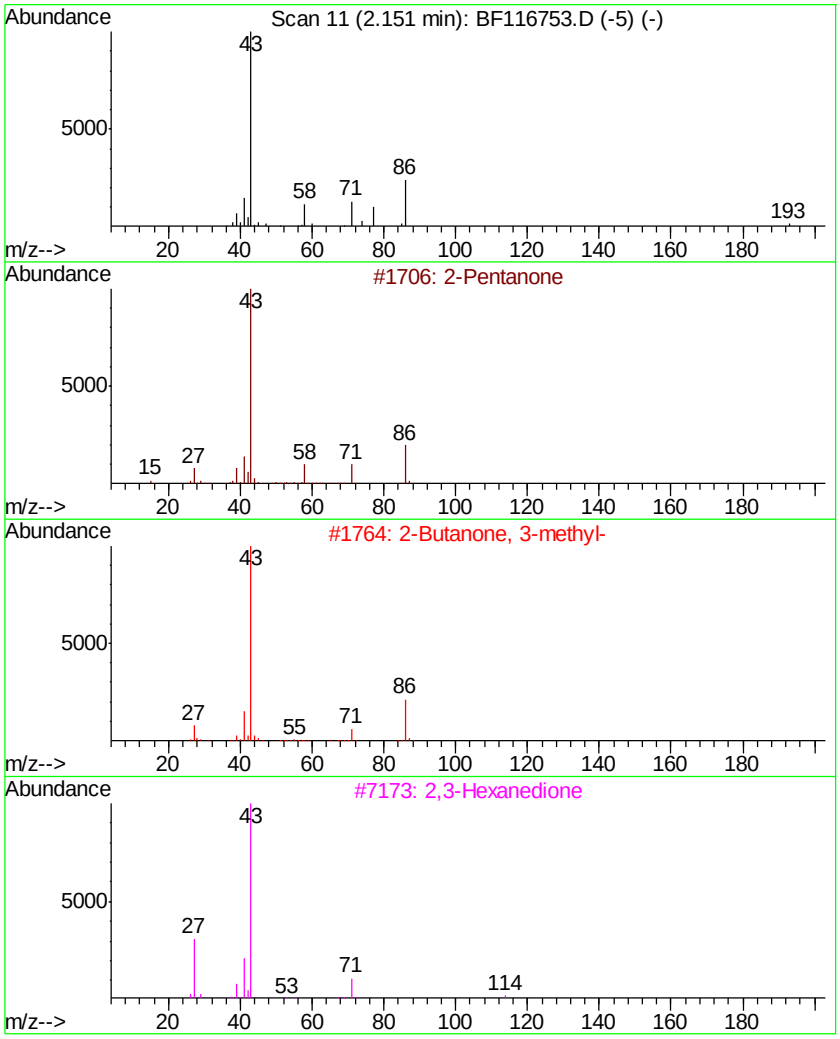
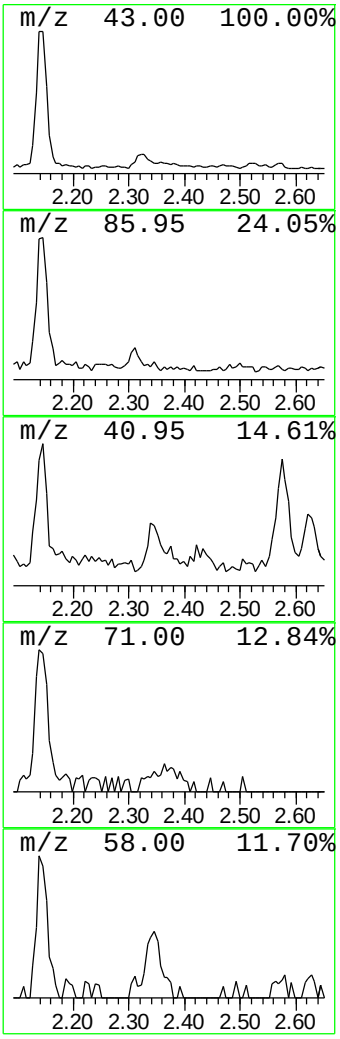
****

Peak Number 1 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	3.41 ng	92180	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	80
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	50
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	9
4	Thioacetic acid	76	C2H4OS	000507-09-5	9
5	Cyclopropylmethanol acetate	114	C6H10O2	036982-54-4	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

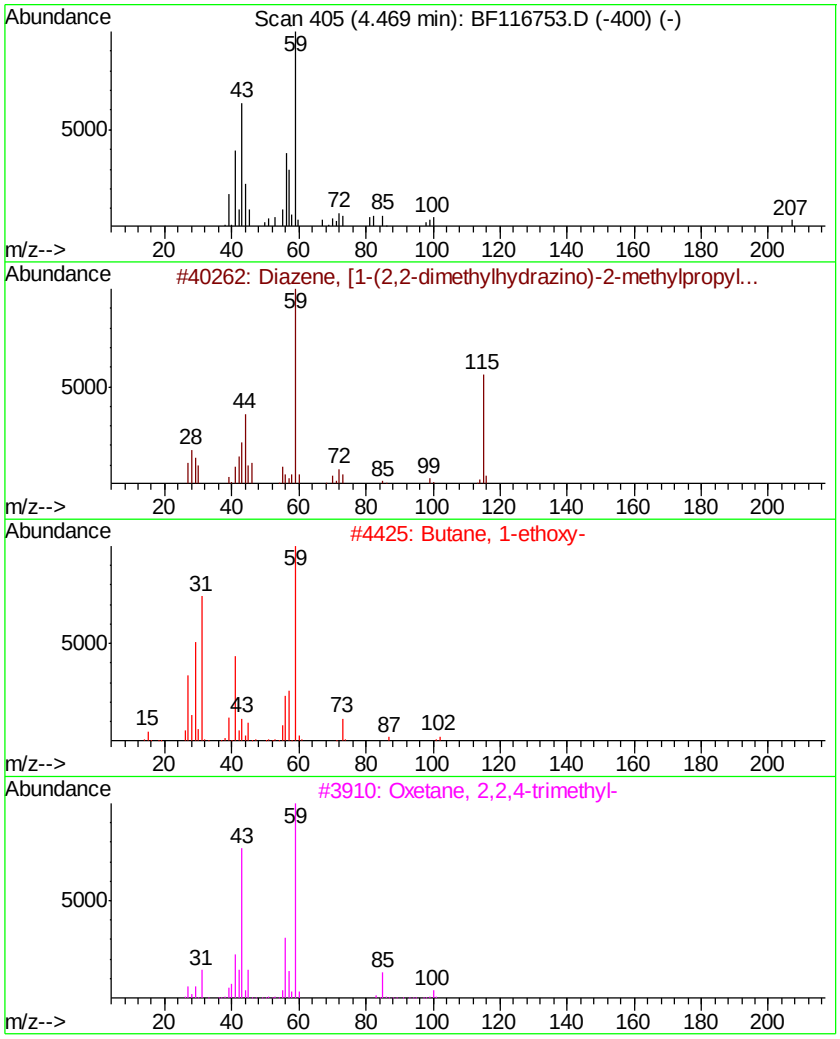
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

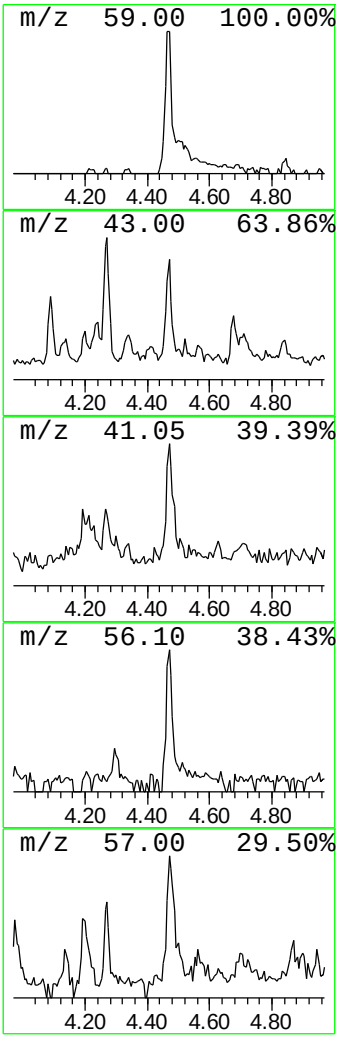
****

Peak Number 2 Diazene, [1-(2,2-dimethylhy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	2.86 ng	77342	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diazene, [1-(2,2-dimethylhydrazi...	172	C8H20N4	061940-94-1	50
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	47
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	45
4	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	45
5	1-(1-Methoxypropan-2-yloxy)propa...	260	C14H28O4	1000367-13-1	43





Library Search Compound Report

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Operator : HP/JU
Sample : K4547-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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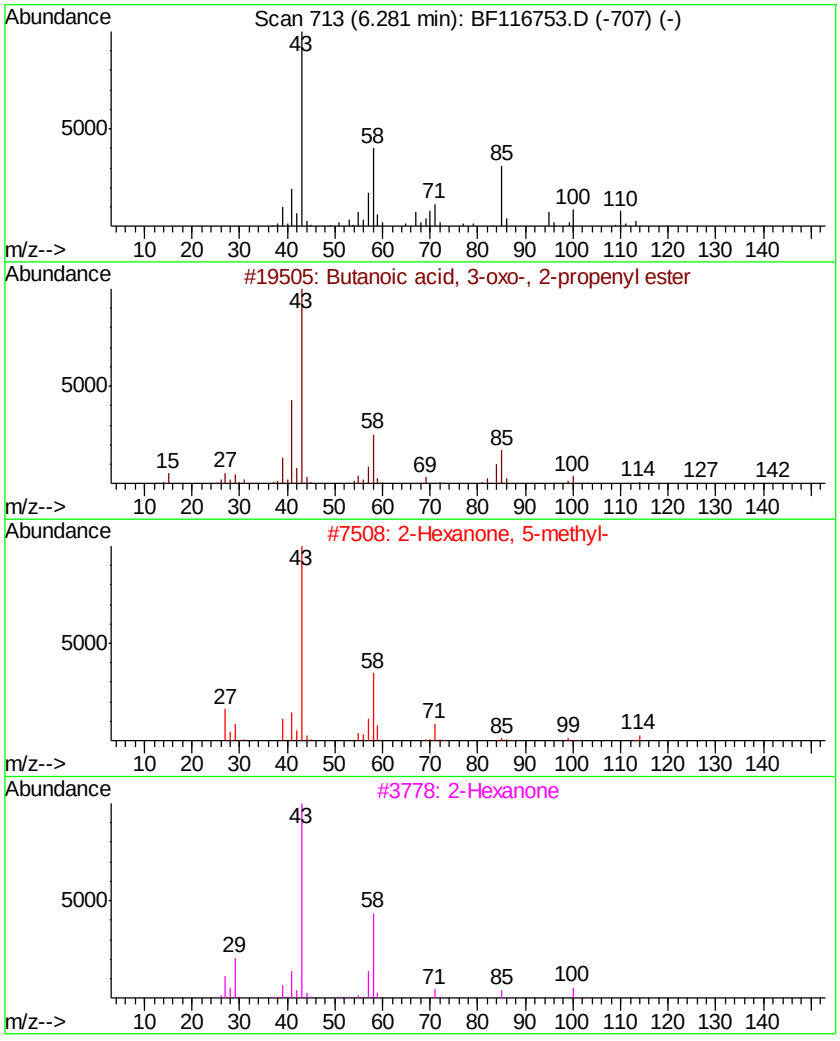
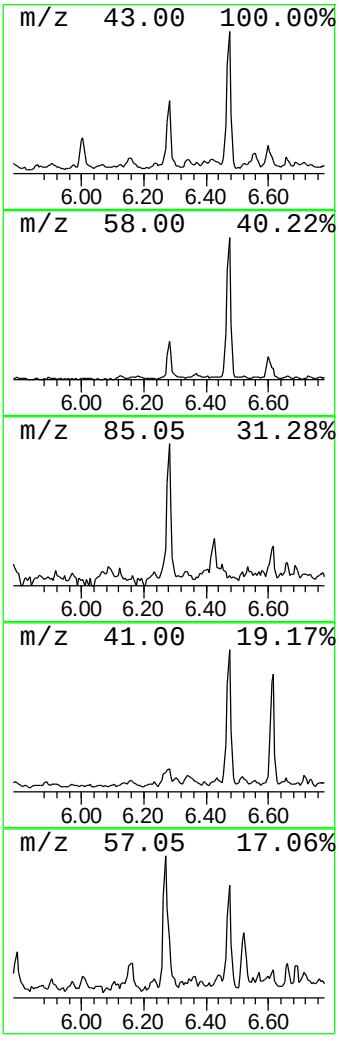
Peak Number 3 Butanoic acid, 3-oxo-, 2-pr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.28	4.08 ng	110268	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-oxo-, 2-propenyl...	142	C7H10O3	001118-84-9	64
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	53
3	2-Hexanone	100	C6H12O	000591-78-6	53
4	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	53
5	2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	42





Library Search Compound Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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TIC Library : C:\DATABASE\NIST11.L
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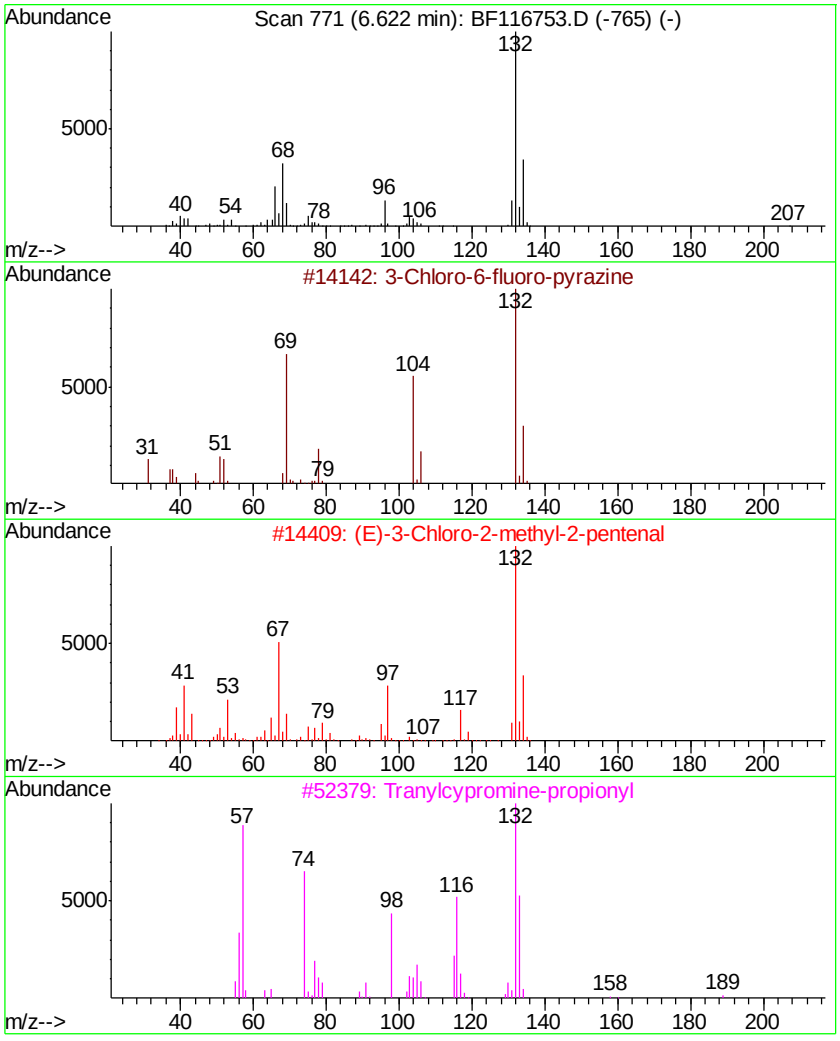
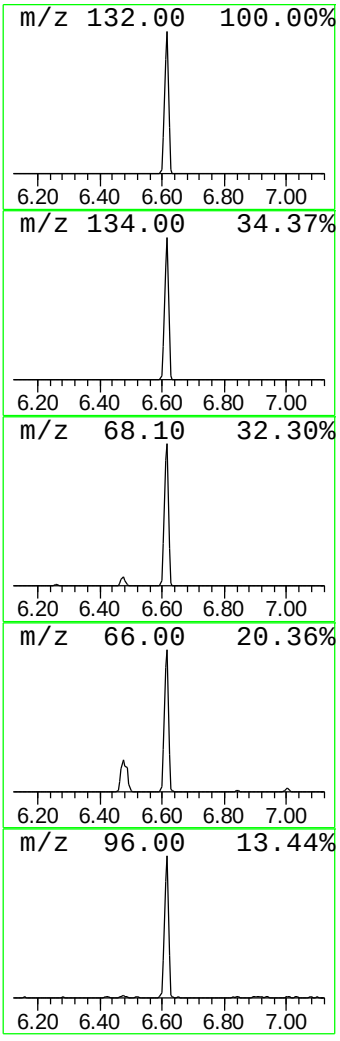
****

Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	68.00 ng	1838420	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : K4547-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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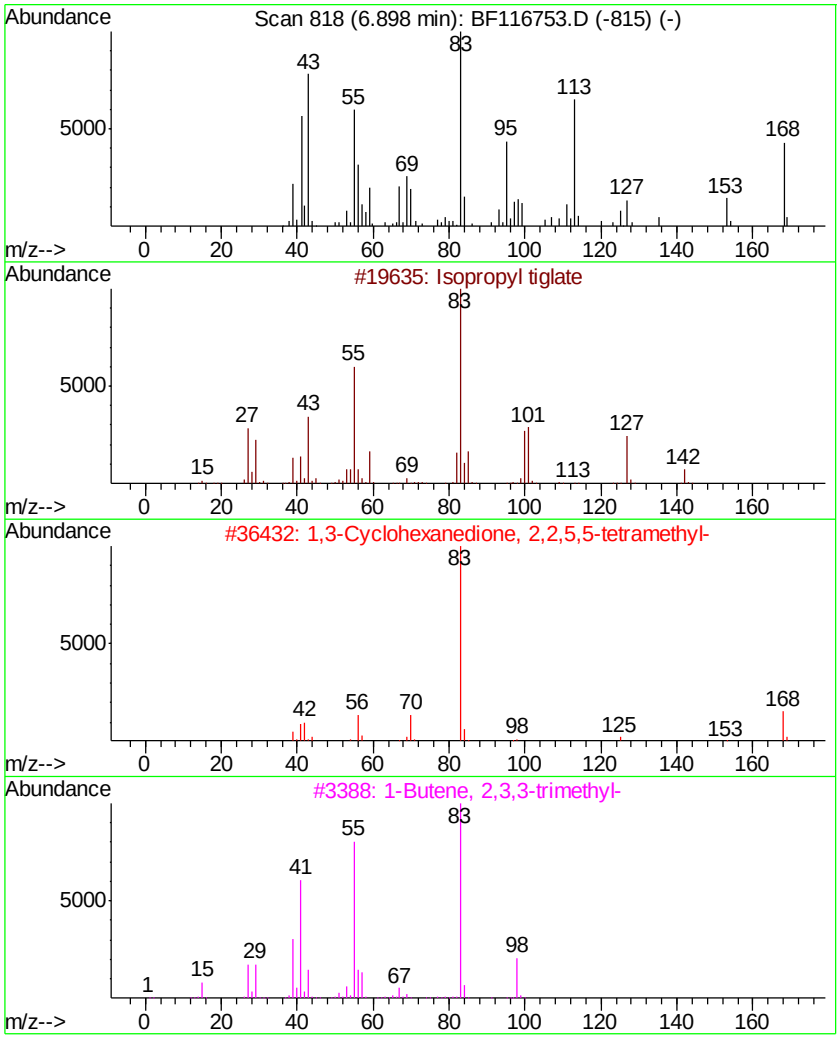
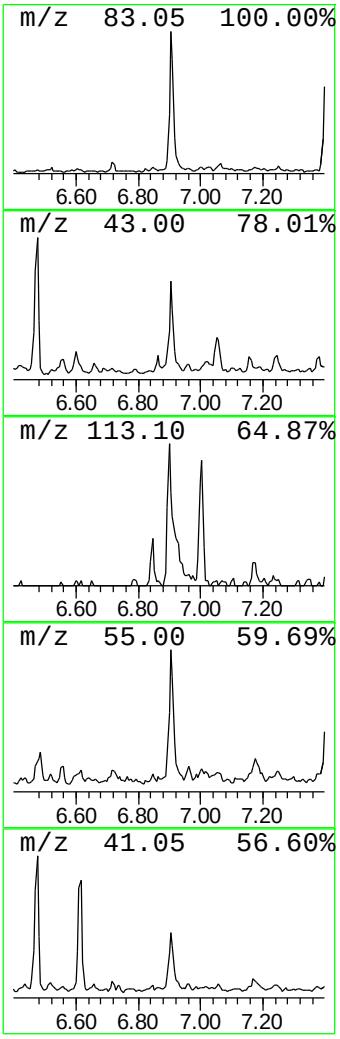
****

Peak Number 5 Isopropyl tiglate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	11.36 ng	307061	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl tiglate	142	C8H14O2	001733-25-1	50
2	1,3-Cyclohexanedione, 2,2,5,5-te...	168	C10H16O2	000702-50-1	50
3	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	43
4	2-Decene, 2,4-dimethyl-	168	C12H24	074421-03-7	43
5	Cyclohexane, hexyl-	168	C12H24	004292-75-5	38





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ClientSampleId : T3-S-F

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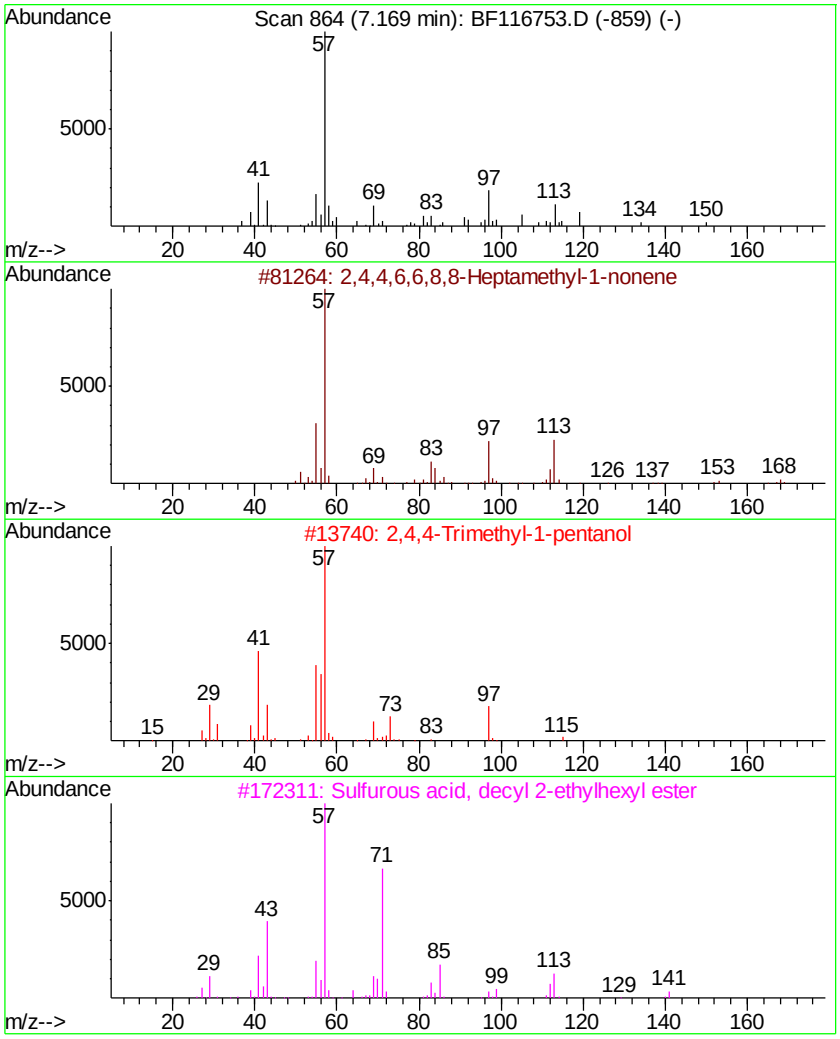
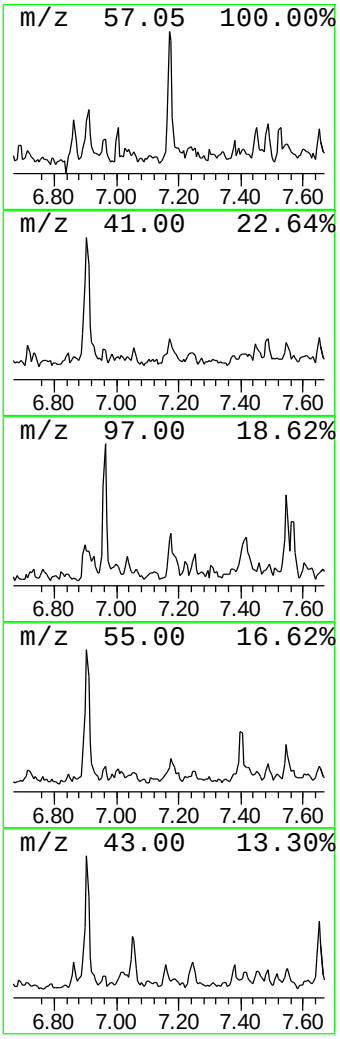
****

Peak Number 7 unknown7.17 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	3.30 ng	89129	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	42
2	2,4,4-Trimethyl-1-pentanol	130	C8H18O	016325-63-6	32
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	28
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27
5	2-Carbamoylaziridine-1-carboxyli...	186	C8H14N2O3	1000185-33-5	25





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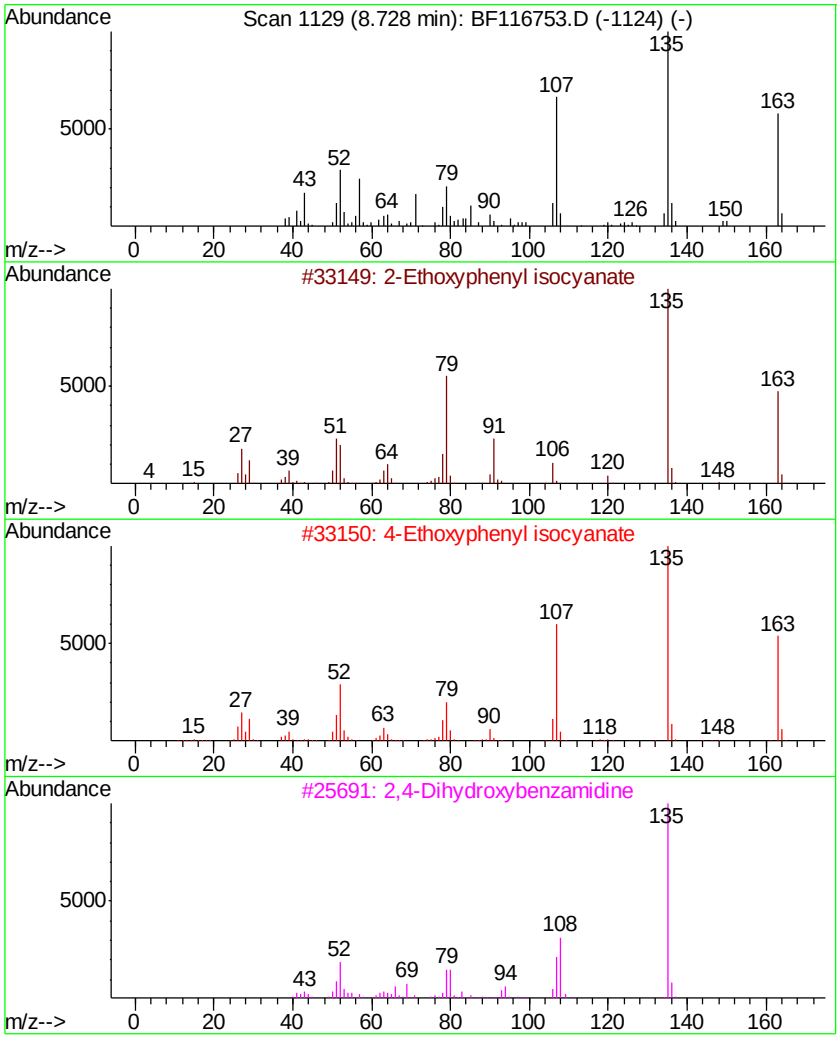
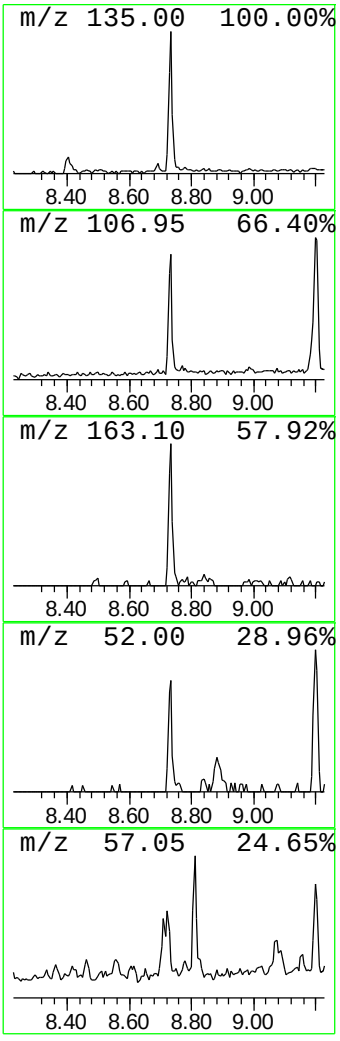
****

Peak Number 8 2-Ethoxyphenyl isocyanate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.71 ng	104050	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethoxyphenyl isocyanate	163	C9H9NO2	005395-71-1	72
2	4-Ethoxyphenyl isocyanate	163	C9H9NO2	032459-62-4	58
3	2,4-Dihydroxybenzamidine	152	C7H8N2O2	1000111-25-6	53
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	50
5	2(3H)-Benzoxazolone	135	C7H5NO2	000059-49-4	47





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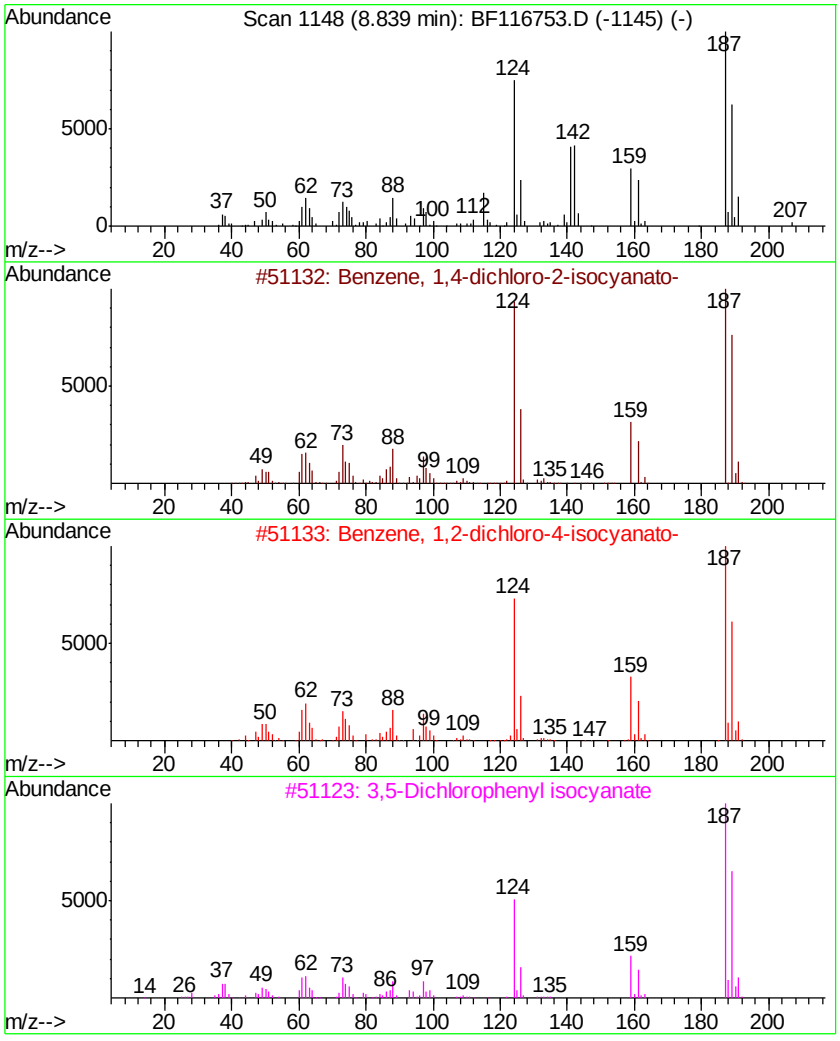
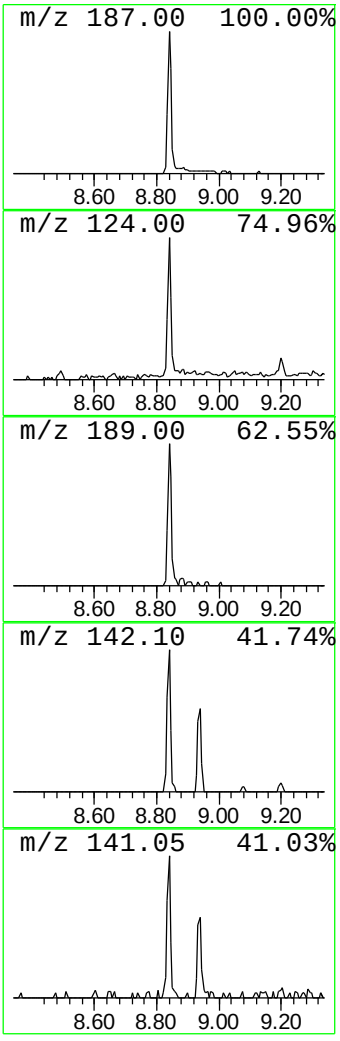
****

Peak Number 9 Benzene, 1,4-dichloro-2-iso... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	3.10 ng	119023	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-dichloro-2-isocyanato-	187	C7H3Cl2NO	005392-82-5	96
2	Benzene, 1,2-dichloro-4-isocyanato-	187	C7H3Cl2NO	000102-36-3	95
3	3,5-Dichlorophenyl isocyanate	187	C7H3Cl2NO	034893-92-0	93
4	Benzene, 1,3-dichloro-2-isocyanato-	187	C7H3Cl2NO	039920-37-1	93
5	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	89





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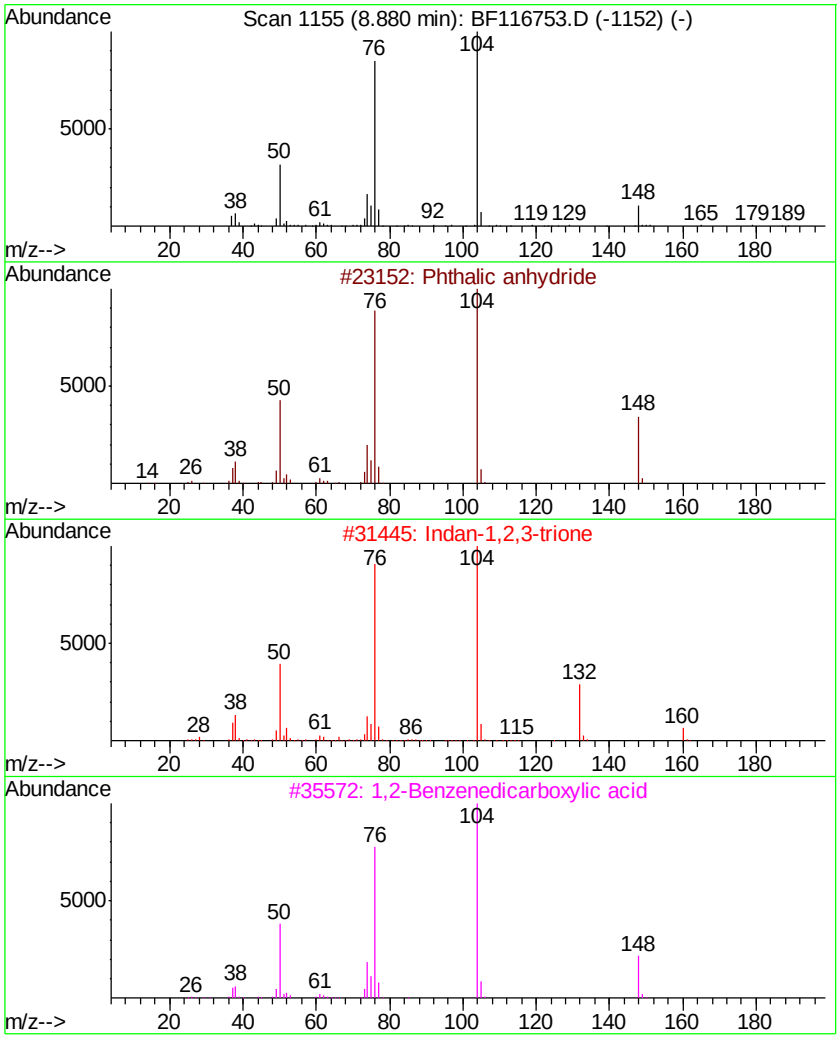
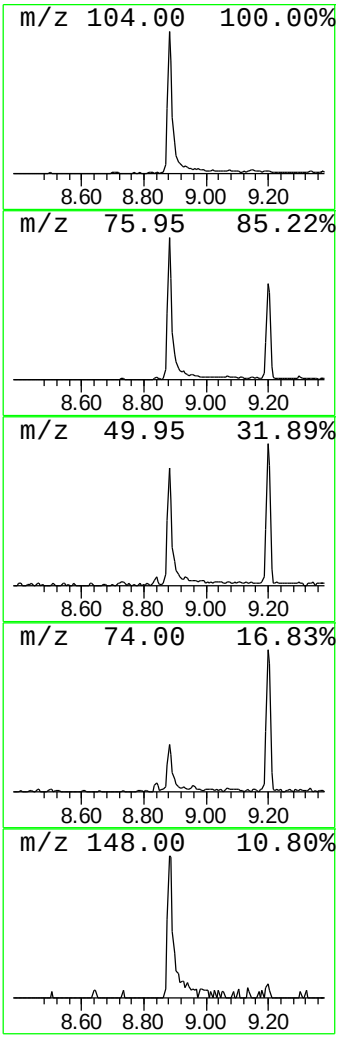
Peak Number 10 Phthalic anhydride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	5.59 ng	214576	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	83
3	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
4	Ninhydrin	178	C9H6O4	000485-47-2	83
5	1H-Isoindole-1,3(2H)-dione, 2-(h...	177	C9H7NO3	000118-29-6	78





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

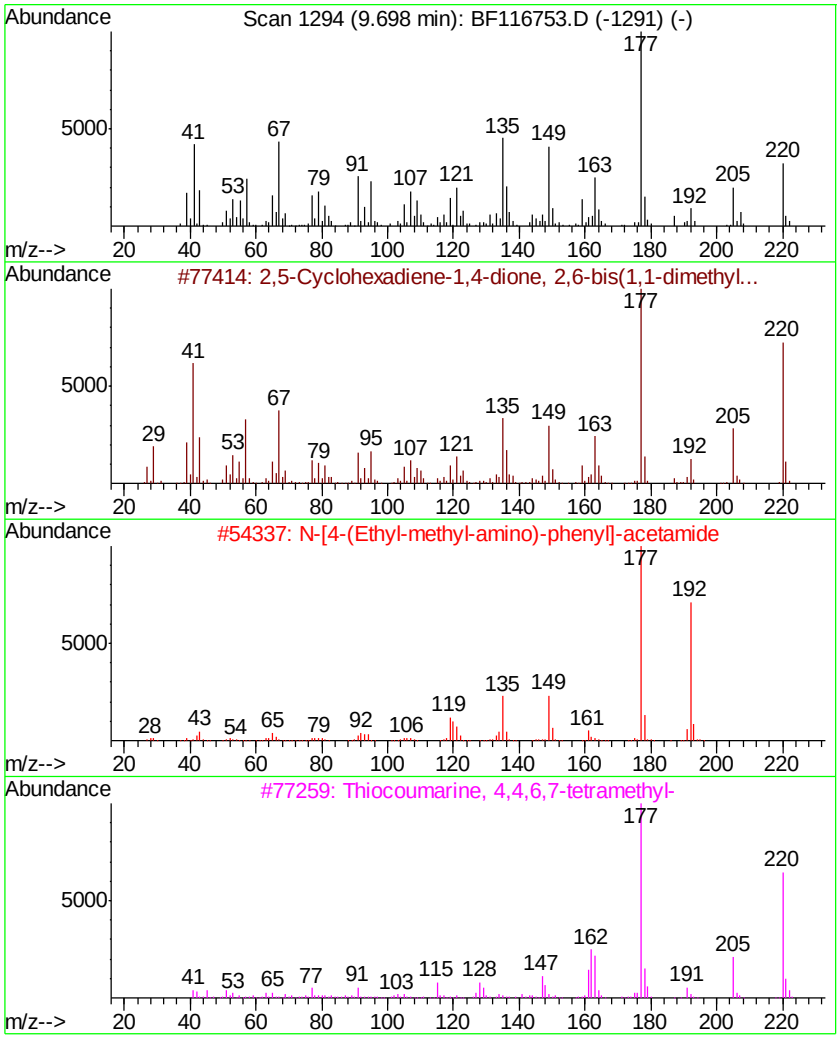
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

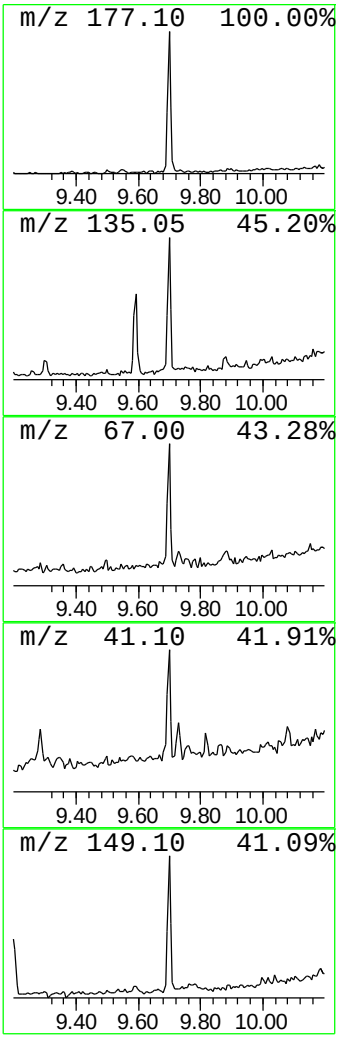
****

Peak Number 11 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	5.02 ng	256293	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	46
3	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	41
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090119\
Data File : BF116753.D
Acq On : 1 Sep 2019 20:03
Operator : HP/JU
Sample : K4547-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone	2.15	3.4	ng	92180	1	6.85	540723	20.0
Diazene, [1-(2,2-...	4.47	2.9	ng	77342	1	6.85	540723	20.0
Butanoic acid, 3-...	6.28	4.1	ng	110268	1	6.85	540723	20.0
unknown6.62	6.62	68.0	ng	1838420	1	6.85	540723	20.0
Isopropyl tiglate	6.90	11.4	ng	307061	1	6.85	540723	20.0
unknown7.17	7.17	3.3	ng	89129	1	6.85	540723	20.0
2-Ethoxyphenyl is...	8.73	2.7	ng	104050	2	8.13	767069	20.0
Benzene, 1,4-dich...	8.84	3.1	ng	119023	2	8.13	767069	20.0
Phthalic anhydride	8.88	5.6	ng	214576	2	8.13	767069	20.0
2,5-Cyclohexadien...	9.70	5.0	ng	256293	3	9.88	1020350	20.0